BIOCHEMISTRY
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SUPPLEMENTARY MATERIAL

Part I: *Proton assignment for the reduced yeast cytochrome c (shift values measured at 303 K).*

7.294	HN	-4	1.705	HB2	11
8.889	HN	-3	2.085	HB3	11
4.489	HA	-3	1.450	HG3	11
2.748	HB3	-3	8.081	HN	12
3.049	HB2	-3	4.419	HA	12
7.146	CG	-3	1.427	QG2	12
7.427	CZ	-3	8.707	HN	13
7.272	HZ	-3	5.208	HA	13
6.742	HN	-2	2.636	HB2	13
3.926	HA	-2	2.353	HB3	13
1.252	HB2	-2	1.952	HG2	13
1.518	HB3	-2	2.246	HG3	13
7.787	HN	-1	3.415	HD2	13
3.779	HA	-1	3.539	HD3	13
1.377	QB	-1	8.069	HN	14
8.268	HN	1	5.310	HA	14
3.603	HA1	1	1.807	HB3	14
4.487	HA2	1	0.944	HB2	14
9.596	HN	2	7.372	HN	15
4.887	HA	2	4.236	HA	15
3.770	HB2	2	1.392	HB2	15
3.967	HB3	2	1.895	HB3	15
4.194	HA	3	1.578	HG	15
1.596	QB	3	1.101	QD1	15
8.379	HN	4	0.965	QD2	15
4.373	HA	4	8.911	HN	16
7.872	HN	5	3.969	HA	16
4.255	HA	5	2.039	HB2	16
8.887	HN	6	2.278	HB3	16
3.643	HA1	6	2.513	HG2	16
4.325	HA2	6	2.775	HG3	16
8.127	HN	7	7.644	HE21	16
2.457	HA	7	7.095	HE22	16
1.245	QB	7	7.033	HN	17
7.309	HN	8	4.312	HA	17
3.983	HA	8	0.644	HB2	17
4.334	HB	8	1.584	HB3	17
1.323	QG2	8	6.689	HN	18
8.093	HN	9	3.602	HA	18
4.183	HA	9	0.755	HB2	18
2.294	HB2	9	1.130	HB3	18
1.443	HB3	9	0.511	HE1	18
1.858	HG	9	0.093	HD2	18
0.917	QD2	9	9.759	HD1	18
1.227	QD1	9	3.543	QM5	18
8.955	HN	10	2.294	QM8	18
4.126	HA	10	3.486	QM1	18
3.066	HB2	10	3.878	QM3	18
3.003	HB3	10	9.178	HDM	18
7.183	CG	10	1.496	QT2	18
6.163	HE1	10	5.229	HT2A	18
6.162	HZ	10	9.348	HAM	18
6.755	HE2	10	2.546	QT4	18
8.387	HN	11	6.392	HT4A	18
4.084	HA	11	3.648	HAP72	18

4.123	HAP71	18
3.369	HBP74	18
2.696	HBP73	18
9.644	HGM	18
9.719	HBM	18
7.347	HN	19
4.532	HA	19
4.365	HB	19
1.040	QG2	19
8.060	HN	20
3.929	HA	20
1.328	HB	20
0.229	QG1	20
0.357	QG2	20
8.399	HN	21
4.159	HA	21
1.824	HB2	21
1.902	HB3	21
8.642	HN	22
3.173	HA	22
1.335	HB3	22
0.600	HB2	22
0.755	HG2	22
0.971	HG3	22
1.443	HD2	22
2.854	HE2	22
9.178	HN	23
3.547	HA1	23
3.903	HA2	23
7.891	HN	24
3.179	HA1	24
4.175	HA	25
2.171	HB2	25
8.402	HN	26
4.428	HA	26
3.093	HB2	26
2.809	HB3	26
7.027	HD2	26
7.574	HE1	26
7.697	HN	27
4.520	HA	27
1.145	HB2	27
1.088	HB3	27
7.053	HN	28
3.986	HA	28
2.039	HB	28
1.778	QG1	28
1.306	QG2	28
7.760	HN	29
3.653	HA1	29
-0.013	HA2	29
3.645	HA	30
0.443	HB3	30
1.262	HB2	30
0.133	HG3	30
0.770	HG2	30
1.900	HD3	30
1.362	HD2	30
10.794	HN	31
4.069	HA	31
2.037	HB2	31
2.150	HB3	31
7.785	HD21	31
7.903	HN	32
3.919	HA	32
0.978	HB2	32
1.291	HB3	32
0.361	HG	32
-0.948	QD1	32
-0.603	QD2	32
7.551	HN	33
3.884	HA	33
2.900	HB2	33
7.080	HD2	33
7.840	HE1	33
9.036	HN	34
7.103	HN	35
3.737	HA	35
1.606	HB	35
0.261	QG2	35
0.957	HG13	35
1.283	HG12	35
0.657	QD1	35
7.835	HN	36
4.389	HA	36
2.976	HB2	36
3.063	HB3	36
7.231	CG	36
6.831	CZ	36
7.105	HZ	36
8.787	HN	37
3.835	HA1	37
4.263	HA2	37
8.073	HN	38
4.856	HA	38
2.040	HB2	38
2.086	HB3	38
2.176	HG2	38
1.850	HG3	38
3.192	HD2	38
3.275	HD3	38
7.958	HN	39
5.564	HA	39
2.941	HB3	39
2.777	HB2	39
6.797	HD2	39
8.010	HE1	39
8.778	HN	40
4.996	HA	40
3.670	HB2	40
3.770	HB3	40
8.237	HN	41
3.490	HA1	41
1.411	HA2	41
8.247	HN	42
4.651	HA	42
1.950	HB2	42
2.290	HG2	42
2.427	HG3	42
6.826	HE22	42
7.523	HE21	42
8.681	HN	43
4.416	HA	43
1.566	QB	43
8.825	HN	44
4.261	HA	44
2.113	HB2	44
2.442	HB3	44

2.366	HG2	44
7.225	HN	46
4.126	HA	46
2.206	HB2	46
1.020	HB3	46
4.788	HD1	46
6.898	HE2	46
6.259	HD2	46
6.992	HN	47
4.561	HA	47
3.692	HB2	47
3.496	HB3	47
8.218	HN	48
5.203	HA	48
2.946	HB2	48
3.783	HB3	48
8.043	HD1	48
7.089	HE1	48
7.217	HE2	48
7.481	HD2	48
9.787	HH	48
10.307	HN	49
4.518	HA	49
4.726	HB	49
1.817	QG2	49
8.616	HG1	49
8.715	HN	50
4.519	HA	50
2.687	HB2	50
2.623	HB3	50
7.756	HN	51
3.975	HA	51
1.369	QB	51
8.271	HN	52
4.174	HA	52
3.199	HB2	52
2.988	HB3	52
7.698	HN	53
3.416	HA	53
1.888	HB	53
0.958	QG2	53
1.935	HG12	53
1.202	HG13	53
1.094	QD1	53
9.098	HN	54
3.930	HA	54
1.755	HB2	54
1.877	HB3	54
1.550	HG2	54
1.469	HG3	54
1.610	HD3	54
7.481	HN	55
3.864	HA	55
1.801	HB2	55
1.892	HB3	55
7.054	HN	56
4.391	HA	56
2.931	HB3	56
2.300	HB2	56
7.684	HD21	56
6.305	HD22	56
7.427	HN	57
3.763	HA	57
1.056	HB	57
0.413	QG1	57
-0.194	QG2	57
8.268	HN	58
3.824	HA	58
1.645	HB3	58
0.835	HB2	58
1.064	HG	58
0.323	QD1	58
0.711	QD2	58
7.991	HN	59
5.041	HA	59
2.693	HB3	59
3.229	HB2	59
7.043	HD1	59
7.641	HE3	59
8.996	HE1	59
6.692	HZ3	59
7.165	HZ2	59
5.729	HH2	59
9.641	HN	60
4.950	HA	60
2.847	HB2	60
3.122	HB3	60
10.266	HN	61
3.719	HA	61
1.561	HB3	61
1.119	HB2	61
8.287	HN	62
4.631	HA	62
2.912	HB2	62
2.982	HB3	62
7.171	HD22	62
7.804	HD21	62
9.587	HN	63
4.554	HA	63
2.853	HB2	63
3.147	HB3	63
7.510	HD21	63
7.000	HD22	63
9.034	HN	64
2.285	HB2	64
2.758	HB3	64
1.285	QE	64
7.858	HN	65
3.970	HA	65
7.819	HN	66
3.848	HA	66
2.336	HB3	66
2.089	HB2	66
8.425	HN	67
3.595	HA	67
3.035	HB2	67
3.112	HB3	67
7.201	HD1	67
7.552	HE1	67
7.750	HE2	67
7.283	HD2	67
8.374	HN	68
3.084	HA	68
1.798	HB2	68
1.226	HB3	68
2.077	HG	68
0.225	QD1	68
1.134	QD2	68

7.387	HN	69
3.903	HA	69
4.182	HB	69
1.110	QG2	69
6.246	HN	70
4.259	HA	70
2.783	HB2	70
2.750	HB3	70
0.879	HB2	71
0.135	HG2	71
0.775	HG3	71
2.771	HD2	71
3.096	HD3	71
7.707	HN	72
3.830	HA	72
1.618	HB2	72
1.677	HB3	72
1.167	HG2	72
3.056	HE2	72
3.189	HE3	72
2.953	QQH	72
7.036	HN	73
4.033	HA	73
1.659	HB3	73
7.382	HN	74
4.269	HA	74
3.158	HB2	74
3.252	HB3	74
7.227	CG	74
6.673	CZ	74
8.320	HN	75
4.115	HA	75
1.962	HB	75
0.614	QG2	75
1.011	QD1	75
4.551	HA	76
1.756	HB2	76
2.221	HB3	76
1.969	HG2	76
0.627	HG3	76
3.182	HD2	76
3.377	HD3	76
8.768	HN	77
3.633	HA1	77
4.282	HA2	77
8.227	HN	78
4.611	HA	78
4.276	HB	78
0.834	QG2	78
8.761	HN	79
4.280	HA	79
7.067	HN	80
3.116	HA	80
-2.434	HB2	80
-0.173	HB3	80
-3.698	HG2	80
-1.776	HG3	80
-3.181	QE	80
8.164	HN	81
4.025	HA	81
1.392	QB	81
6.250	HN	82
4.469	HA	82
0.606	HB2	82
2.047	HB3	82
6.752	CG	82
7.450	CZ	82
7.169	HZ	82
8.738	HN	84
3.038	HA1	84
4.256	HA2	84
8.459	HN	85
4.729	HA	85
1.524	HB2	85
1.636	HB3	85
1.845	HG	85
1.097	QD1	85
1.175	QD2	85
8.687	HN	86
4.009	HA	86
1.827	HB2	86
8.890	HN	87
4.475	HA	87
1.908	HB2	87
1.856	HB3	87
1.777	HG2	87
9.084	HN	88
3.634	HA	88
2.006	HB2	88
2.126	HB3	88
8.779	HN	89
4.036	HA	89
1.895	HB2	89
1.739	HB3	89
1.520	HG2	89
1.607	HG3	89
6.530	HN	90
4.413	HA	90
2.673	HB2	90
3.013	HB3	90
7.618	HN	91
3.944	HA	91
2.222	HB2	91
1.942	HB3	91
1.209	HG2	91
1.746	HG3	91
8.837	HN	92
4.038	HA	92
2.852	HB2	92
3.070	HB3	92
7.360	HD21	92
7.168	HD22	92
8.833	HN	93
4.336	HA	93
2.713	HB2	93
2.812	HB3	93
8.663	HN	94
4.352	HA	94
2.093	HB2	94
2.241	HB3	94
1.528	QD1	94
1.240	QD2	94
9.304	HN	95
3.730	HA	95
2.226	HB	95
0.655	QG2	95
2.177	HG12	95
1.113	QD1	95

8.312	HN	96	3.629	HA	99
3.947	HA	96	1.444	HB2	99
4.537	HB	96	1.646	HB3	99
1.310	QG2	96	6.768	HN	100
7.997	HN	97	4.198	HA	100
4.212	HA	97	1.850	HB2	100
3.726	HB2	97	1.456	HB3	100
3.222	HB3	97	8.445	HN	101
6.948	CG	97	3.948	HA	101
6.282	CZ	97	0.588	QB	101
9.406	HN	98	7.717	HN	102
3.426	HA	98	4.307	HA	102
1.857	HB2	98	6.881	HN	103
1.907	HB3	98	4.061	HA	103
0.875	QD1	98	2.350	HB2	103
0.953	QD2	98	2.009	HB3	103
8.890	HN	99			

Part II: *Experimental NOESY intensities used for the structure calculation of reduced yeast iso-1-cytochrome c.*
(The figures of the volumes come from the computer output; their last digits do not have physical meaning. However, the empirical calibration procedures of CALIBA and the use of only upper distance limits remove any effect of these meaningless digits in the following structure calculations.)

-4 Glu					
	HN	-3	Phe	HN	4317.0
-3 Phe					
	HN	-3	Phe	HA	1279.0
	HN	-3	Phe	HB3	1367.0
	HA	-3	Phe	HB2	3096.9
	HA	-3	Phe	HB3	1102.5
	HA	-3	Phe	CG	1801.5*2
	HA	-2	Lys	HN	835.0
	HA	92	Asn	HD22	249.0
	HB2	-3	Phe	CG	1457.0*2
	HB2	-3	Phe	CZ	506.7*2
	HB3	-3	Phe	CG	2204.5*2
	CG	-3	Phe	CZ	6345.0*2*2
	CG	-2	Lys	HA	164.5*2
	CG	61	Glu	HB2	75.0*2
	CG	61	Glu	HB3	430.6*2
	CG	92	Asn	HA	79.5*2
	CG	95	Ile	HB	1687.0*2
	CG	95	Ile	QG2	660.5*2
	CG	95	Ile	QD1	311.0*2
	CG	96	Thr	HN	181.0*2
	CZ	-3	Phe	HZ	9080.0*2
	CZ	61	Glu	HB3	391.9*2
	CZ	92	Asn	HB3	120.1*2
	CZ	95	Ile	HN	116.0*2
	CZ	95	Ile	HA	71.5*2

	CZ	95 Ile	HB	1971.0*2
	CZ	95 Ile	QG2	1073.5*2
	CZ	95 Ile	QD1	334.8*2
	CZ	96 Thr	HN	308.5*2
	HZ	-1 Ala	HA	2075.0
	HZ	-1 Ala	QB	1619.0
	HZ	1 Gly	HN	1222.0
	HZ	95 Ile	HB	551.7
	HZ	95 Ile	QG2	802.0
	HZ	96 Thr	HN	602.0
	HZ	96 Thr	HA	1810.8
-2 Lys				
	HN	-2 Lys	HA	4146.0
	HN	-2 Lys	HB2	2413.0
	HN	-2 Lys	HB3	3916.0
	HN	92 Asn	HB3	834.0
	HN	92 Asn	HD21	374.0
	HN	92 Asn	HD22	905.0
	HA	-2 Lys	HB2	3256.0
	HA	-2 Lys	HB3	2143.0
	HA	-1 Ala	HN	5469.0
	HB2	-1 Ala	HN	439.0
	HB3	-1 Ala	HN	1363.0
-1 Ala				
	HN	-1 Ala	HA	1639.0
	HN	-1 Ala	QB	10220.0
	HA	-1 Ala	QB	8853.0
	HA	1 Gly	HN	5616.0
	HA	92 Asn	HB3	632.0
	HA	96 Thr	QG2	495.0
	QB	1 Gly	HN	7986.0
1 Gly				
	HN	1 Gly	HA1	766.0
	HN	1 Gly	HA2	1878.0
	HN	2 Ser	HN	943.0
	HN	93 Asp	HA	244.0
	HN	96 Thr	QG2	1817.0
	HA1	2 Ser	HN	2660.0
	HA1	93 Asp	HA	1073.0
	HA2	2 Ser	HN	893.0
2 Ser				
	HN	2 Ser	HB2	1234.0
	HN	2 Ser	HB3	151.0
	HN	93 Asp	HA	754.0
	HN	93 Asp	HB2	202.0
	HA	2 Ser	HB2	9522.0
	HA	2 Ser	HB3	5094.9
3 Ala				
	HA	3 Ala	QB	7920.0
	HA	4 Lys	HN	3681.0
	HA	6 Gly	HN	157.0
	HA	96 Thr	QG2	1293.0
	QB	97 Tyr	CG	395.1*2
4 Lys				
	HN	4 Lys	HA	1329.0

	HA	5	Lys	HN	3697.0
5 Lys					
	HN	5	Lys	HA	912.0
	HN	6	Gly	HN	1976.0
	HA	6	Gly	HN	337.0
	HA	7	Ala	HN	421.0
	HA	8	Thr	HN	153.0
6 Gly					
	HN	6	Gly	HA1	2335.0
	HN	6	Gly	HA2	619.0
	HN	7	Ala	HN	3741.0
	HN	7	Ala	QB	988.0
	HN	93	Asp	HB2	897.0
	HN	97	Tyr	HB2	601.0
	HA1	7	Ala	HN	529.0
	HA1	10	Phe	HN	250.0
	HA1	93	Asp	HB2	252.0
	HA1	93	Asp	HB3	268.0
	HA2	7	Ala	HN	1499.0
	HA2	9	Leu	HN	673.0
	HA2	97	Tyr	HB3	1312.0
7 Ala					
	HN	7	Ala	HA	5100.0
	HN	7	Ala	QB	16490.0
	HN	8	Thr	HN	3273.0
	HN	97	Tyr	HB2	494.0
	HA	7	Ala	QB	10330.0
	HA	8	Thr	HN	1647.0
	HA	10	Phe	HN	984.0
	HA	10	Phe	HB2	1030.0
	HA	10	Phe	HB3	960.0
	HA	11	Lys	HN	965.0
	HA	97	Tyr	CG	291.5*2
	QB	8	Thr	HN	3673.0
	QB	97	Tyr	CG	1861.6*2
	QB	97	Tyr	CZ	910.8*2
8 Thr					
	HN	8	Thr	HA	2474.0
	HN	8	Thr	HB	7009.0
	HN	8	Thr	QG2	1482.0
	HN	9	Leu	HN	3073.0
	HA	8	Thr	HB	6465.0
	HA	8	Thr	QG2	10360.0
	HA	9	Leu	HN	678.0
	HA	11	Lys	HN	849.0
	HA	11	Lys	HB2	377.0
	HA	11	Lys	HB3	4028.0
	HB	8	Thr	QG2	8210.0
	HB	9	Leu	HN	192.0
	QG2	9	Leu	HN	2159.0
9 Leu					
	HN	9	Leu	HA	1952.0
	HN	9	Leu	HB2	5158.0
	HN	9	Leu	HB3	2910.0
	HN	10	Phe	HN	4584.0
	HN	11	Lys	HN	1717.0

HA	9	Leu	HB2	2731.0
HA	9	Leu	HB3	1938.0
HA	9	Leu	HG	8527.0
HA	9	Leu	QD1	1280.0
HA	9	Leu	QD2	3598.2
HA	10	Phe	HN	766.0
HA	13	Arg	HG2	649.0
HB2	9	Leu	QD1	4981.0
HB2	9	Leu	QD2	1284.0
HB2	10	Phe	HN	4152.0
HB2	94	Leu	QD1	1758.0
HB3	10	Phe	HN	1282.0
HB3	10	Phe	HA	511.0
HG	9	Leu	QD1	4835.0
HG	10	Phe	HN	578.0
QD1	90	Asp	HA	3528.0
QD1	90	Asp	HB2	2184.0
QD1	90	Asp	HB3	2958.3
QD1	93	Asp	HN	888.0
QD1	94	Leu	HN	1708.0

10 Phe

HN	10	Phe	HA	2285.0
HN	10	Phe	HB2	3981.0
HN	10	Phe	HB3	4070.0
HN	11	Lys	HN	4858.0
HN	94	Leu	QD1	4878.0
HN	94	Leu	QD2	765.0
HA	10	Phe	HB2	960.0
HA	10	Phe	HB3	3746.7
HA	10	Phe	CG	2365.5*2
HA	14	Cys	HN	459.0
HA	94	Leu	QD1	2680.0
HA	94	Leu	QD2	1559.0
HB2	10	Phe	CG	2984.0*2
HB2	94	Leu	QD1	2171.0
HB3	10	Phe	CG	1539.5*2
HB3	11	Lys	HN	2211.0
HB3	94	Leu	QD1	1620.0
HB3	97	Tyr	CG	1248.3*2
HB3	97	Tyr	CZ	484.2*2
CG	10	Phe	HE1	588.0*2
CG	10	Phe	HE2	7370.0*2
CG	11	Lys	HN	642.5*2
CG	11	Lys	HA	912.1*2
CG	15	Leu	HB2	911.7*2
CG	15	Leu	QD1	1407.0*2
CG	15	Leu	QD2	1317.5*2
CG	32	Leu	QD1	137.5*2
CG	94	Leu	QD1	4438.5*2
CG	98	Leu	QD1	498.6*2
HE1	15	Leu	HA	424.0
HE1	15	Leu	HB2	225.0
HE1	15	Leu	QD1	1705.0
HE1	15	Leu	QD2	1493.0
HE1	19	Thr	HA	274.5
HE1	20	Val	QG2	453.0
HE1	98	Leu	QD1	546.0
HZ	18	Hes	HB2	2334.0
HZ	18	Hes	HB3	2312.0
HZ	19	Thr	HA	202.5

	HZ	20	Val	QG1	3210.0
	HZ	20	Val	QG2	1276.0
	HZ	32	Leu	QD1	2931.0
	HE2	15	Leu	QD1	2491.0
	HE2	18	Hes	QM1	575.0
	HE2	20	Val	QG1	1956.0
	HE2	32	Leu	HG	320.0
	HE2	32	Leu	QD1	6268.0
	HE2	98	Leu	QD2	4561.0
11	Lys				
	HN	11	Lys	HA	2844.0
	HN	11	Lys	HB2	4900.0
	HN	11	Lys	HB3	4539.0
	HN	11	Lys	HG3	1303.0
	HN	12	Thr	HN	2393.0
	HN	15	Leu	QD2	1223.0
	HA	11	Lys	HB2	3256.0
	HA	11	Lys	HB3	3005.0
	HA	11	Lys	HG3	2036.0
	HA	12	Thr	HN	482.0
	HA	15	Leu	HN	562.0
	HA	15	Leu	HB2	3113.0
	HA	15	Leu	QD1	12006.0
	HA	15	Leu	QD2	4917.0
	HB2	12	Thr	HN	315.0
	HB3	11	Lys	HG3	1903.0
	HB3	12	Thr	HN	3083.0
12	Thr				
	HN	12	Thr	HA	1641.0
	HN	12	Thr	QG2	3468.0
	HA	12	Thr	QG2	9779.0
	HA	13	Arg	HA	495.0
	HA	13	Arg	HG3	615.0
13	Arg				
	HN	13	Arg	HA	1447.0
	HN	13	Arg	HB3	1681.0
	HN	13	Arg	HG2	1074.0
	HN	13	Arg	HG3	286.0
	HN	13	Arg	HD2	191.0
	HN	14	Cys	HN	10260.0
	HN	15	Leu	HN	310.0
	HA	13	Arg	HB2	3250.8
	HA	13	Arg	HB3	9776.0
	HA	13	Arg	HG2	681.0
	HA	13	Arg	HG3	1510.0
	HA	13	Arg	HD2	1961.0
	HA	13	Arg	HD3	3047.0
	HA	14	Cys	HN	411.0
	HA	14	Cys	HA	160.0
	HA	82	Phe	CZ	632.2*2
	HB2	13	Arg	HG2	472.0
	HB2	14	Cys	HN	1025.0
	HB2	18	Hes	QT2	1666.0
	HB2	82	Phe	CZ	587.7*2
	HB2	85	Leu	QD1	2364.3
	HB2	85	Leu	QD2	981.0
	HB3	13	Arg	HD2	3360.0
	HB3	13	Arg	HD3	2332.0

	HB3	82 Phe	CG	70.0*2
	HB3	82 Phe	CZ	1264.5*2
	HG2	13 Arg	HD3	8617.0
	HG3	13 Arg	HD2	4517.0
	HD2	82 Phe	CZ	1009.3*2
	HD3	82 Phe	CZ	120.1*2
14 Cys				
	HN	14 Cys	HA	745.0
	HN	14 Cys	HB2	1294.0
	HN	14 Cys	HB3	900.0
	HN	15 Leu	HN	7858.0
	HN	15 Leu	HB3	256.0
	HA	14 Cys	HB2	2529.0
	HA	14 Cys	HB3	3116.0
	HA	18 Hes	HD2	623.0
	HA	18 Hes	HT2A	1519.0
	HA	18 Hes	QT2	937.0
	HA	18 Hes	HAM	2281.0
	HA	18 Hes	QM3	1619.0
	HB2	15 Leu	HN	1013.0
	HB2	18 Hes	QM1	4931.0
	HB2	18 Hes	HT2A	391.5
	HB3	18 Hes	HD2	1714.0
	HB3	18 Hes	HT2A	1118.0
	HB3	18 Hes	HAM	613.8
15 Leu				
	HN	15 Leu	HA	1095.0
	HN	15 Leu	HB2	4512.0
	HN	15 Leu	HB3	2023.0
	HN	15 Leu	HG	286.0
	HN	16 GLN	HN	1231.0
	HA	15 Leu	HB2	823.0
	HA	15 Leu	HB3	4216.0
	HA	15 Leu	HG	2867.0
	HA	15 Leu	QD1	3591.0
	HA	15 Leu	QD2	215.0
	HA	16 GLN	HN	498.0
	HA	17 Cys	HN	304.0
	HA	18 Hes	HN	1651.0
	HB2	15 Leu	QD1	4560.0
	HB3	15 Leu	QD2	19030.0
	HG	15 Leu	QD2	6423.0
16 GLN				
	HN	16 GLN	HA	4176.0
	HN	16 GLN	HB2	1573.0
	HN	16 GLN	HB3	2081.0
	HN	16 GLN	HG2	3068.0
	HN	17 Cys	HN	1995.0
	HA	16 GLN	HB2	6791.0
	HA	16 GLN	HB3	6308.0
	HA	16 GLN	HG2	762.0
	HA	16 GLN	HG3	559.0
	HB2	16 GLN	HG3	3024.0
	HB2	18 Hes	QM3	2684.0
	HB3	16 GLN	HG3	15660.0
	HB3	16 GLN	HE21	558.0
	HG2	16 GLN	HE21	1141.0
	HG2	16 GLN	HE22	1151.0

	HG2	17	Cys	HN	1503.0
	HG2	17	Cys	HB2	921.0
	HG2	18	Hes	HN	255.0
	HG3	16	GLN	HE22	659.0
	HG3	17	Cys	HN	1433.0
	HG3	18	Hes	HN	622.0

17 Cys

	HN	17	Cys	HA	2072.0
	HN	17	Cys	HB2	3104.0
	HN	17	Cys	HB3	1186.0
	HN	18	Hes	HN	9045.0
	HN	18	Hes	HB2	556.0
	HN	18	Hes	QM3	732.0
	HA	17	Cys	HB2	826.0
	HA	18	Hes	HN	347.0
	HA	28	Val	HN	375.0
	HA	28	Val	HB	6718.0
	HA	29	Gly	HN	445.0
	HB2	18	Hes	HN	759.0
	HB2	18	Hes	HD2	404.0
	HB2	18	Hes	HT4A	908.0
	HB2	18	Hes	HBM	426.0
	HB2	29	Gly	HN	471.0
	HB3	18	Hes	HN	2840.0
	HB3	18	Hes	HAM	348.3
	HB3	18	Hes	HT4A	2479.0
	HB3	18	Hes	HBM	1184.0
	HB3	28	Val	HN	500.0
	HB3	29	Gly	HN	933.0

18 Hes

	HN	18	Hes	HA	2104.0
	HN	18	Hes	HB2	3553.0
	HN	18	Hes	HB3	1400.0
	HN	18	Hes	HD2	446.0
	HN	19	Thr	HN	322.0
	HA	18	Hes	HB2	2137.0
	HA	18	Hes	HB3	2120.0
	HA	18	Hes	HD1	928.0
	HA	19	Thr	HN	6138.0
	HB2	18	Hes	HD1	650.0
	HB2	18	Hes	HD2	1560.0
	HB2	32	Leu	QD1	1736.0
	HB3	18	Hes	HD1	1640.0
	HB3	18	Hes	HD2	417.6
	HB3	19	Thr	HN	627.0
	HB3	32	Leu	HN	243.0
	HB3	32	Leu	QD1	2575.8
	HB3	32	Leu	QD2	524.0
	HD1	18	Hes	HD2	224.0
	HD1	18	Hes	HE1	3762.0
	HD1	19	Thr	HN	132.0
	HD1	29	Gly	HA2	506.0
	HD1	30	Pro	HB2	154.0
	HD1	30	Pro	HG2	657.0
	HD1	32	Leu	HB2	112.0
	HD1	32	Leu	HG	3779.0
	HD1	32	Leu	QD1	2059.0
	HD1	32	Leu	QD2	2631.0
	HD2	18	Hes	HE1	727.0

HD2	18	Hes	HT2A	183.6
HD2	18	Hes	HAM	338.0
HD2	18	Hes	QM3	141.0
HD2	32	Leu	QD1	674.0
HE1	18	Hes	HGM	371.0
HE1	29	Gly	HA1	272.0
HE1	29	Gly	HA2	549.0
HE1	30	Pro	HD2	4400.0
HE1	30	Pro	HD3	1661.0
HE1	32	Leu	QD1	475.2
HE1	32	Leu	QD2	1646.0
HAP71	18	Hes	HBP74	6099.0
HAP71	18	Hes	HGM	763.0
HAP72	18	Hes	HBP73	1262.0
HAP72	18	Hes	QM8	8232.0
HAP72	18	Hes	HGM	412.0
HAP72	32	Leu	QD2	279.0
HAP72	48	Tyr	HE1	207.0
HAP72	59	Trp	HZ2	3594.6
HAP72	59	Trp	HH2	389.7
HBP73	18	Hes	HBP74	10100.0
HBP73	18	Hes	HGM	1668.0
HBP73	30	Pro	HG2	3258.0
HBP73	32	Leu	QD2	2082.0
HBP74	18	Hes	HGM	718.0
HBP74	30	Pro	HG2	869.0
HBP74	32	Leu	HG	218.7
HBP74	32	Leu	QD2	2914.0
HBP74	48	Tyr	HE1	1436.4
QM8	18	Hes	HDM	7197.0
QM8	18	Hes	QM1	516.0
QM8	18	Hes	HGM	135.9
QM8	32	Leu	QD1	1010.0
QM8	32	Leu	QD2	4923.0
QM8	35	Ile	QG2	1655.0
QM8	35	Ile	HG12	5552.0
QM8	35	Ile	QD1	2018.0
[illegible]				

HDM	18	Hes	QM1	9503.0
HDM	18	Hes	QT2	407.0
HDM	32	Leu	HB3	158.0
HDM	32	Leu	QD1	3010.0
HDM	32	Leu	QD2	924.0
HDM	68	Leu	QD1	1798.0
HDM	68	Leu	QD2	463.0
HDM	80	Met	QE	242.0
HDM	98	Leu	QD1	429.3
HDM	98	Leu	QD2	649.8
QM1	18	Hes	HT2A	175.5
QM1	18	Hes	QT2	4872.0
QM1	32	Leu	QD1	4071.0
QM1	32	Leu	QD2	498.0
QM1	68	Leu	QD1	7760.7
QM1	68	Leu	QD2	6237.0

	HT2A	80	Met	QE	421.2
	HT2A	82	Phe	CG	157.1*2
	QT2	18	Hes	HAM	2532.0
	QT2	68	Leu	QD1	4218.0
	QT2	80	Met	QE	1128.0
	QT2	82	Phe	CZ	2777.0*2
	QT2	82	Phe	HZ	3228.0
	HAM	18	Hes	QM3	4221.0
	HAM	80	Met	QE	691.0
	HAM	82	Phe	HB3	234.9
	HAM	82	Phe	CG	240.8*2
	QM3	18	Hes	HT4A	270.0
	QM3	18	Hes	QT4	8091.0
	QM3	82	Phe	HB2	1593.0
	QM3	82	Phe	CG	515.5*2
	HT4A	18	Hes	QT4	9344.0
	HT4A	18	Hes	HBM	16250.0
	HT4A	18	Hes	QM5	1271.0
	HT4A	28	Val	HB	917.0
	HT4A	28	Val	QG1	8289.0
	HT4A	28	Val	QG2	150.0
	HT4A	80	Met	HA	110.7
	HT4A	81	Ala	HN	260.0
	QT4	18	Hes	HBM	2732.0
	QT4	28	Val	QG1	3224.0
	QT4	81	Ala	HN	2063.0
	QT4	81	Ala	QB	5143.0
	QT4	82	Phe	HB3	1996.0
	HBM	18	Hes	QM5	6289.0
	HBM	28	Val	HB	555.3
	HBM	28	Val	QG1	5910.0
	HBM	80	Met	HA	1131.0
	HBM	81	Ala	HN	616.0
	HBM	81	Ala	QB	74.0
	QM5	28	Val	QG1	11040.0
	QM5	29	Gly	HA2	701.0
	QM5	80	Met	HB2	345.6
	HGM	30	Pro	HG2	133.0
	HGM	30	Pro	HD2	222.3
	HGM	30	Pro	HD3	287.1
	HGM	32	Leu	QD2	120.0
19 Thr					
	HN	19	Thr	HA	344.0
	HN	19	Thr	QG2	128.0
	HN	31	Asn	HA	721.0
	HN	32	Leu	HN	766.0
	HA	19	Thr	HB	28593.0
	HA	19	Thr	QG2	683.0
	HA	20	Val	HN	7952.0
	HA	20	Val	QG1	460.8
	HA	21	Glu	HN	1191.0
	HB	19	Thr	QG2	10980.0
	HB	20	Val	HN	731.0
	QG2	20	Val	HN	729.0
	QG2	21	Glu	HN	241.0
20 Val					
	HN	20	Val	HA	730.0
	HN	20	Val	HB	932.0
	HN	20	Val	QG1	4176.0

	HN	20	Val	QG2	2837.0
	HN	21	Glu	HN	5972.0
	HN	21	Glu	HB3	256.0
	HA	20	Val	QG1	3198.0
	HA	20	Val	QG2	5479.0
	HB	20	Val	QG1	5002.0
	HB	20	Val	QG2	5589.0
	HB	21	Glu	HN	806.0
	HB	32	Leu	QD1	185.4
	HB	101	Ala	QB	7236.9
	QG1	21	Glu	HN	2661.0
	QG1	21	Glu	HA	448.2
	QG1	32	Leu	HN	278.0
	QG1	97	Tyr	CG	108.0*2
	QG1	97	Tyr	CZ	124.2*2
	QG1	98	Leu	QD1	1327.5
	QG1	98	Leu	QD2	5891.0
	QG1	101	Ala	QB	2674.8
	QG2	21	Glu	HN	743.0
	QG2	21	Glu	HA	428.4
	QG2	21	Glu	HB3	673.2
	QG2	97	Tyr	CZ	50.8*2
	QG2	101	Ala	QB	11240.0
21 Glu					
	HN	21	Glu	HA	1007.0
	HN	21	Glu	HB3	3599.0
	HA	21	Glu	HB2	5718.0
	HA	21	Glu	HB3	16821.0
	HA	22	Lys	HN	3948.0
	HB2	22	Lys	HN	2696.0
	HB3	22	Lys	HN	4273.0
	HB3	24	Gly	HA1	804.0
22 Lys					
	HN	22	Lys	HA	1772.0
	HN	22	Lys	HB2	3890.0
	HN	22	Lys	HB3	3151.0
	HN	22	Lys	HG2	213.0
	HN	22	Lys	HG3	410.0
	HN	33	HIS	HE1	294.0
	HA	22	Lys	HB2	5811.0
	HA	22	Lys	HB3	4444.0
	HA	22	Lys	HG2	4042.0
	HA	22	Lys	HG3	2548.0
	HA	22	Lys	HD2	958.0
	HA	23	Gly	HN	1948.0
	HA	24	Gly	HN	1688.0
	HA	33	HIS	HD2	732.6
	HB2	22	Lys	HD2	3089.0
	HB2	22	Lys	HE2	596.0
	HB2	23	Gly	HN	130.0
	HB2	33	HIS	HD2	580.5
	HB2	33	HIS	HE1	367.2
	HB3	22	Lys	HG2	475.2
	HB3	22	Lys	HE2	1147.0
	HG2	22	Lys	HE2	2116.0
	HG2	23	Gly	HN	734.0
	HG2	33	HIS	HE1	220.0
	HG3	22	Lys	HE2	2827.8
	HD2	22	Lys	HE2	3716.0

	HD2	33 HIS	HD2	961.2
	HD2	33 HIS	HE1	543.6
	HE2	33 HIS	HE1	228.6
23 Gly				
	HN	23 Gly	HA1	1257.0
	HN	23 Gly	HA2	114.0
	HN	24 Gly	HN	769.0
	HA1	24 Gly	HN	746.0
24 Gly				
	HN	24 Gly	HA1	1512.0
	HA1	31 Asn	HD21	718.0
25 Pro				
	HA	25 Pro	HB2	2046.0
	HA	26 HIS	HN	2026.0
	HB2	26 HIS	HN	2204.0
26 HIS				
	HN	26 HIS	HA	949.0
	HN	26 HIS	HB2	2289.0
	HN	26 HIS	HB3	275.0
	HA	26 HIS	HB2	3958.2
	HA	26 HIS	HB3	7751.7
	HA	27 Lys	HN	518.0
	HA	30 Pro	HA	1672.2
	HA	31 Asn	HN	351.0
	HA	31 Asn	HB2	179.0
	HB2	26 HIS	HD2	2825.1
	HB2	27 Lys	HN	857.0
	HB2	30 Pro	HA	3424.5
	HB3	27 Lys	HN	433.0
	HB3	31 Asn	HN	545.0
	HB3	46 Tyr	HE2	391.5
	HB3	46 Tyr	HD2	210.0
	HD2	26 HIS	HE1	715.0
	HD2	46 Tyr	HA	160.0
	HD2	46 Tyr	HB2	1046.7
	HD2	46 Tyr	HB3	405.9
	HE1	30 Pro	HA	143.1
	HE1	30 Pro	HB2	157.5
	HE1	30 Pro	HB3	346.5
	HE1	31 Asn	HN	1716.0
	HE1	31 Asn	HB2	1375.0
	HE1	31 Asn	HB3	752.0
	HE1	43 Ala	QB	4981.0
	HE1	46 Tyr	HB2	808.2
	HE1	46 Tyr	HB3	176.4
27 Lys				
	HN	27 Lys	HA	1685.0
	HN	27 Lys	HB2	3806.0
	HN	27 Lys	HB3	1999.0
	HN	30 Pro	HA	507.0
	HA	27 Lys	HB3	5906.0
	HB2	28 Val	HN	7895.0
	HB2	29 Gly	HN	1108.0
	HB3	28 Val	HN	1906.0
28 Val				

	HN	28	Val	HA	2179.0
	HN	28	Val	HB	6032.0
	HN	28	Val	QG2	5408.0
	HN	29	Gly	HN	1467.0
	HA	28	Val	HB	3561.0
	HA	28	Val	QG1	6456.0
	HA	28	Val	QG2	8126.0
	HB	28	Val	QG1	55580.0
	HB	28	Val	QG2	7589.0
	HB	29	Gly	HN	4211.0
	QG1	29	Gly	HN	3389.0
	QG1	29	Gly	HA1	1066.0
	QG2	29	Gly	HN	1188.0
29 Gly					
	HN	29	Gly	HA1	1247.0
	HN	29	Gly	HA2	2932.0
	HA2	30	Pro	HD2	788.0
	HA2	30	Pro	HD3	781.0
30 Pro					
	HA	30	Pro	HB2	5414.0
	HA	30	Pro	HB3	8253.0
	HA	30	Pro	HG2	3876.0
	HA	30	Pro	HG3	2328.0
	HA	31	Asn	HN	5688.0
	HB2	31	Asn	HN	531.0
	HB3	30	Pro	HG3	3123.0
	HB3	31	Asn	HN	185.0
	HB3	46	Tyr	HD1	237.6
	HB3	46	Tyr	HD2	147.0
	HG2	30	Pro	HD3	3225.0
	HG2	32	Leu	QD2	6921.0
	HG2	48	Tyr	HE1	3094.2
	HG2	48	Tyr	HE2	2363.0
	HD2	46	Tyr	HD2	120.6
	HD3	48	Tyr	HE2	489.0
31 Asn					
	HN	31	Asn	HA	1222.0
	HN	31	Asn	HB2	3517.0
	HN	31	Asn	HB3	2477.0
	HN	43	Ala	QB	272.0
	HA	31	Asn	HB2	4467.0
	HA	31	Asn	HB3	2262.0
	HA	31	Asn	HD21	1235.0
	HA	32	Leu	HN	8604.0
	HA	32	Leu	HG	609.3
	HA	33	HIS	HN	694.0
	HB3	31	Asn	HD21	1705.0
	HB3	32	Leu	HN	1795.0
32 Leu					
	HN	32	Leu	HA	4321.0
	HN	32	Leu	HB2	3451.0
	HN	32	Leu	HB3	1585.0
	HN	32	Leu	HG	3347.0
	HN	32	Leu	QD1	1118.0
	HN	32	Leu	QD2	721.0
	HN	33	HIS	HN	7858.0
	HA	32	Leu	HB2	4698.0

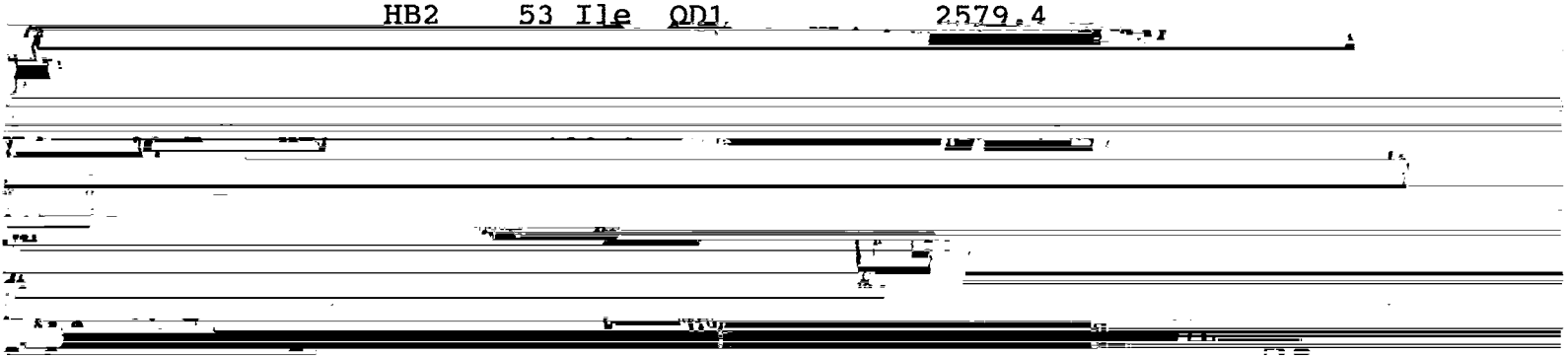
	HA	32	Leu	QD1	706.0
	HA	32	Leu	QD2	6259.0
	HA	33	HIS	HN	1316.0
	HB2	32	Leu	HG	7984.0
	HB2	32	Leu	QD1	5852.0
	HB2	32	Leu	QD2	3074.0
	HB2	35	Ile	QG2	3003.0
	HB3	32	Leu	QD1	3039.3
	HB3	32	Leu	QD2	6127.0
	HG	32	Leu	QD1	11470.0
	HG	32	Leu	QD2	7251.0
	QD1	35	Ile	QG2	2208.0
	QD1	98	Leu	QD1	2083.0
	QD2	35	Ile	HB	1380.0
	QD2	35	Ile	QG2	1919.0
	QD2	35	Ile	QD1	2083.0
33 HIS					
	HN	33	HIS	HA	829.0
	HN	33	HIS	HB2	6509.0
	HA	33	HIS	HB2	3445.0
	HA	33	HIS	HD2	87.0
	HA	34	Gly	HN	3260.0
	HA	102	Ser	HA	1363.0
	HB2	33	HIS	HD2	2686.5
	HB2	34	Gly	HN	924.0
	HD2	33	HIS	HE1	3913.0
	HD2	34	Gly	HN	238.0
34 Gly					
	HN	35	Ile	HN	2086.0
	HN	35	Ile	QG2	349.0
	HN	35	Ile	QD1	368.0
35 Ile					
	HN	35	Ile	HA	7371.0
	HN	35	Ile	HB	1126.0
	HN	35	Ile	QG2	7666.0
	HN	35	Ile	HG12	642.0
	HN	35	Ile	HG13	2480.0
	HN	35	Ile	QD1	4635.0
	HA	35	Ile	HB	5002.0
	HA	35	Ile	QG2	1707.0
	HA	35	Ile	HG12	810.0
	HA	35	Ile	QD1	1840.0
	HA	36	Phe	HN	1306.0
	HA	38	Arg	HG3	545.0
	HB	35	Ile	QG2	5296.0
	HB	35	Ile	HG12	2382.0
	HB	35	Ile	QD1	2096.0
	QG2	35	Ile	HG12	3724.0
	QG2	35	Ile	QD1	3758.0
	QG2	36	Phe	HN	5122.0
	QG2	36	Phe	CG	1386.0*2
	QG2	36	Phe	CZ	701.0*2
	QG2	59	Trp	HD1	159.3
	HG12	35	Ile	QD1	6489.0
	HG12	36	Phe	HN	585.0
	HG12	36	Phe	CZ	520.5*2
	HG12	59	Trp	HB3	2716.0
	QD1	36	Phe	HN	299.0

	QD1	36	Phe	CZ	874.0*2
36 Phe					
	HN	36	Phe	HA	5165.0
	HN	36	Phe	HB2	2269.0
	HN	36	Phe	HB3	978.0
	HN	36	Phe	CG	3297.0*2
	HN	37	Gly	HN	1255.0
	HA	36	Phe	HB2	296.0
	HA	36	Phe	HB3	1325.0
	HA	36	Phe	CG	2476.0*2
	HA	37	Gly	HN	1263.0
	HB2	36	Phe	CG	1293.5*2
	HB2	37	Gly	HN	2478.0
	HB2	60	Asp	HA	153.0
	HB3	36	Phe	CG	1969.0*2
	CG	36	Phe	CZ	2927.5*2*2
	CG	36	Phe	HZ	9780.0*2
	CG	37	Gly	HN	813.0*2
	CG	60	Asp	HA	1936.5*2
	CG	61	Glu	HA	163.5*2
	CG	64	Met	QE	141.0*2
	CG	98	Leu	HB3	2402.5*2
	CG	99	Lys	HA	1741.5*2
	CZ	36	Phe	HZ	5270.0*2
	CZ	60	Asp	HA	116.5*2
	CZ	61	Glu	HN	145.5*2
	CZ	61	Glu	HA	1443.0*2
	CZ	61	Glu	HB2	686.5*2
	CZ	64	Met	HB2	333.4*2
	CZ	64	Met	QE	385.6*2
	CZ	98	Leu	HA	58.5*2
	CZ	98	Leu	HB2	2206.0*2
	CZ	98	Leu	HB3	1735.5*2
	CZ	98	Leu	QD2	1178.0*2
	CZ	99	Lys	HN	168.5*2
	CZ	99	Lys	HA	1796.5*2
	HZ	61	Glu	HA	454.5
	HZ	64	Met	HB2	433.8
	HZ	64	Met	HB3	1469.7
	HZ	64	Met	QE	788.4
	HZ	95	Ile	HG12	1327.5
	HZ	98	Leu	HB2	494.0
	HZ	98	Leu	HB3	386.0
	HZ	98	Leu	QD1	450.0
	HZ	99	Lys	HA	474.0
37 Gly					
	HN	37	Gly	HA1	2805.0
	HN	37	Gly	HA2	867.0
	HN	38	Arg	HN	2472.0
	HN	58	Leu	HG	294.0
	HN	58	Leu	QD1	550.0
	HN	58	Leu	QD2	225.0
	HN	59	Trp	HN	598.0
	HA1	38	Arg	HN	747.0
	HA2	58	Leu	QD1	551.0
38 Arg					
	HN	38	Arg	HA	3319.0
	HN	38	Arg	HB2	4036.0

	HN	38	Arg	HB3	995.0
	HN	38	Arg	HG2	1909.0
	HN	58	Leu	QD1	219.0
	HA	38	Arg	HB2	2728.8
	HA	38	Arg	HB3	5347.8
	HA	38	Arg	HG2	2672.1
	HA	38	Arg	HG3	859.5
	HA	38	Arg	HD2	252.0
	HA	38	Arg	HD3	3130.2
	HA	39	HIS	HN	7768.0
	HA	39	HIS	HA	319.5
	HA	39	HIS	HB2	196.0
	HA	58	Leu	QD1	1394.1
	HA	58	Leu	QD2	147.6
	HB2	38	Arg	HD2	870.0
	HB2	38	Arg	HD3	1039.0
	HB2	39	HIS	HN	2580.0
	HB3	38	Arg	HD2	1859.0
	HB3	38	Arg	HD3	1940.0
	HB3	39	HIS	HN	1371.0
	HG2	38	Arg	HD2	3488.0
	HG2	38	Arg	HD3	1776.0
	HG2	39	HIS	HN	2538.0
	HG3	39	HIS	HN	174.0
	HG3	42	GLN	HG2	12710.0
	HG3	59	Trp	HD1	238.5
39 HIS					
	HN	39	HIS	HA	1012.0
	HN	39	HIS	HB2	2434.0
	HN	39	HIS	HB3	394.0
	HN	42	GLN	HE22	702.0
	HA	39	HIS	HB2	4125.0
	HA	39	HIS	HB3	3770.0
	HA	39	HIS	HD2	1063.8
	HA	40	Ser	HN	4611.0
	HA	58	Leu	HA	8526.0
	HA	58	Leu	HB2	679.5
	HA	58	Leu	HB3	180.0
	HA	58	Leu	HG	84.6
	HA	58	Leu	QD1	1991.0
	HA	58	Leu	QD2	273.0
	HA	59	Trp	HN	1475.0
	HA	59	Trp	HD1	222.3
	HB2	39	HIS	HD2	1421.1
	HB3	40	Ser	HN	982.0
	HB3	56	Asn	HD22	505.0
	HD2	39	HIS	HE1	428.0
	HD2	56	Asn	HA	597.6
	HD2	56	Asn	HB3	277.2
	HD2	56	Asn	HD21	512.0
	HD2	58	Leu	HN	400.0
	HD2	58	Leu	HA	871.2
	HD2	58	Leu	HB2	1035.0
	HD2	58	Leu	QD1	1260.0
	HE1	58	Leu	QD1	677.7
40 Ser					
	HN	40	Ser	HA	1140.0
	HN	40	Ser	HB3	1019.0
	HN	56	Asn	HA	1912.0

	HN	57	Val	HN	1488.0
	HN	57	Val	QG1	164.0
	HN	57	Val	QG2	1217.0
	HN	59	Trp	HD1	231.0
	HA	40	Ser	HB3	6801.3
	HA	41	Gly	HN	6337.0
	HA	57	Val	QG2	1098.9
	HA	59	Trp	HD1	1433.0
	HA	59	Trp	HE1	3047.0
	HB2	59	Trp	HE1	845.0
	HB2	59	Trp	HZ2	762.0
	HB3	57	Val	QG1	2617.2
	HB3	57	Val	QG2	3285.0
	HB3	59	Trp	HD1	100.0
	HB3	59	Trp	HE1	498.0
	HB3	59	Trp	HZ2	2980.8
41 Gly					
	HN	41	Gly	HA1	2081.0
	HN	41	Gly	HA2	489.0
	HN	59	Trp	HE1	549.0
	HN	59	Trp	HZ2	848.0
	HA1	42	GLN	HG2	552.0
	HA1	48	Tyr	HE2	899.1
	HA1	53	Ile	HN	360.0
	HA2	43	Ala	HN	2504.0
42 GLN					
	HN	42	GLN	HA	2211.0
	HN	42	GLN	HB2	3371.0
	HN	42	GLN	HG2	549.0
	HN	42	GLN	HG3	2385.0
	HN	43	Ala	HN	4378.0
	HN	48	Tyr	HE2	297.0
	HA	42	GLN	HB2	6889.5
	HA	42	GLN	HG2	7269.0
	HA	42	GLN	HG3	2294.0
	HA	43	Ala	HN	796.0
	HG2	42	GLN	HE21	2200.0
	HG2	42	GLN	HE22	852.0
	HG3	42	GLN	HE21	1892.0
	HG3	42	GLN	HE22	668.0
	HG3	43	Ala	HN	380.0
43 Ala					
	HN	43	Ala	HA	1500.0
	HN	43	Ala	QB	8987.0
	HN	48	Tyr	HE1	167.0
	HN	48	Tyr	HE2	1256.0
	HN	48	Tyr	HH	923.0
	HA	43	Ala	QB	2243.0
	HA	44	Glu	HN	3640.0
	QB	44	Glu	HN	2865.0
	QB	46	Tyr	HD1	558.0
	QB	48	Tyr	HE2	3444.0
	QB	48	Tyr	HD2	478.0
	QB	48	Tyr	HH	1365.0
44 Glu					
	HN	44	Glu	HA	1041.0
	HN	44	Glu	HB2	11420.0

	HN	44	Glu	HB3	1900.0
	HN	44	Glu	HG2	888.0
	HA	44	Glu	HB2	3842.0
	HA	44	Glu	HB3	2367.0
	HA	44	Glu	HG2	1873.8
	HA	46	Tyr	HN	855.0
46 Tyr					
	HN	46	Tyr	HA	851.0
	HN	46	Tyr	HB2	2766.0
	HN	46	Tyr	HB3	4693.0
	HA	46	Tyr	HB2	3006.9
	HA	46	Tyr	HD2	964.8
	HA	47	Ser	HN	448.0
	HB2	46	Tyr	HD1	3279.6
	HB2	46	Tyr	HD2	603.0
	HB3	46	Tyr	HD2	634.0
	HD1	46	Tyr	HE2	2102.4
	HE2	46	Tyr	HD2	17890.0
	HE2	48	Tyr	HA	597.0
	HD2	47	Ser	HN	1885.0
	HD2	48	Tyr	HA	1350.9
	HD2	48	Tyr	HB2	335.0
	HD2	48	Tyr	HD2	141.0
47 Ser					
	HN	47	Ser	HB2	829.0
	HN	47	Ser	HB3	599.0
	HA	47	Ser	HB2	14373.0
	HA	47	Ser	HB3	2565.0
	HA	48	Tyr	HN	1916.0
	HB2	48	Tyr	HN	961.0
48 Tyr					
	HN	48	Tyr	HA	1425.0
	HN	48	Tyr	HB2	3232.0
	HN	48	Tyr	HB3	1112.0
	HN	49	Thr	HN	321.0
	HA	48	Tyr	HB2	328.0
	HA	48	Tyr	HB3	2043.9
	HA	48	Tyr	HD1	606.6
	HA	48	Tyr	HD2	385.2
	HA	49	Thr	HN	3249.0
	HA	53	Ile	QD1	220.5
	HB2	48	Tyr	HD1	1565.1
	HB2	48	Tyr	HD2	858.0
	HB2	49	Thr	HN	1184.0
	HB2	53	Ile	QD1	2579.4



	HD1	48	Tyr	HE1	1384.2
	HD1	48	Tyr	HE2	880.0
	HD1	49	Thr	HN	128.0
	HE1	48	Tyr	HH	656.0
	HE2	48	Tyr	HH	741.0
	HD2	53	Ile	QD1	592.0

	HN	49 Thr	QG2	4003.0
	HN	49 Thr	HG1	806.0
	HN	52 Asn	HN	966.0
	HN	52 Asn	HB3	297.0
	HA	49 Thr	QG2	8976.0
	HB	49 Thr	QG2	10340.0
	HB	51 Ala	QB	2030.4
	QG2	49 Thr	HG1	3054.0
	QG2	50 Asp	HN	3334.0
	QG2	52 Asn	HN	592.0
	QG2	78 Thr	HA	3996.9
	QG2	79 Lys	HN	888.0
	HG1	51 Ala	QB	401.0
	HG1	52 Asn	HN	1694.0
	HG1	52 Asn	HB3	105.0
	HG1	78 Thr	HA	1192.0
50 Asp				
	HN	50 Asp	HA	1848.0
	HN	50 Asp	HB2	6566.0
	HN	50 Asp	HB3	3933.0
	HN	51 Ala	HN	1784.0
	HA	50 Asp	HB2	3959.0
	HA	50 Asp	HB3	5879.0
	HA	51 Ala	HN	3031.0
	HA	53 Ile	HB	1215.0
	HA	53 Ile	QG2	527.0
	HB2	51 Ala	HN	955.0
	HB3	51 Ala	HN	630.0
51 Ala				
	HN	51 Ala	HA	3069.0
	HN	51 Ala	QB	11200.0
	HN	52 Asn	HN	2943.0
	HN	52 Asn	HB2	1137.0
	HA	51 Ala	QB	16686.0
	HA	52 Asn	HN	862.0
	HA	54 Lys	HN	456.0
	QB	75 Ile	QG2	6657.0
	QB	77 Gly	HA1	1208.0
	QB	78 Thr	HN	3622.0
	QB	78 Thr	HA	4082.4
	QB	78 Thr	HB	421.0
52 Asn				
	HN	52 Asn	HA	1100.0
	HN	52 Asn	HB2	1177.0
	HN	52 Asn	HB3	2174.0
	HN	53 Ile	HN	3770.0
	HN	53 Ile	HB	370.0
	HN	54 Lys	HN	377.0
	HN	75 Ile	QG2	748.0
	HA	52 Asn	HB2	2007.0
	HA	52 Asn	HB3	2656.8
	HA	55 Lys	HN	133.0
	HA	55 Lys	HB3	296.0
	HA	75 Ile	QG2	2953.0
	HA	75 Ile	QD1	7405.0
	HB2	78 Thr	HA	629.1
	HB3	75 Ile	QG2	1144.8

53 Ile

	HN	53 Ile	HA	2687.0
	HN	53 Ile	HB	6868.0
	HN	53 Ile	QG2	1572.0
	HN	53 Ile	HG12	3297.0
	HN	53 Ile	QD1	3332.0
	HN	54 Lys	HN	2716.0
	HA	53 Ile	HB	5354.0
	HA	53 Ile	QG2	4151.0
	HA	53 Ile	HG12	3795.0
	HA	53 Ile	HG13	4459.0
	HA	53 Ile	QD1	1564.0
	HA	54 Lys	HN	806.0
	HA	55 Lys	HN	2580.0
	HB	53 Ile	QG2	15777.0
	HB	53 Ile	QD1	13400.0
	HB	54 Lys	HN	5291.0
	QG2	53 Ile	QD1	8645.0
	QG2	54 Lys	HN	1958.0
	QG2	54 Lys	HG3	18660.0
	HG12	53 Ile	QD1	9947.0

54 Lys

	HN	54 Lys	HA	3065.0
	HN	54 Lys	HB2	4319.0
	HN	54 Lys	HG2	1745.0
	HN	54 Lys	HG3	1474.0
	HN	54 Lys	HD3	449.0
	HN	55 Lys	HN	3381.0
	HN	56 Asn	HN	124.0
	HA	54 Lys	HB2	4240.0
	HA	54 Lys	HB3	3158.0
	HA	54 Lys	HG2	1286.0
	HA	54 Lys	HG3	973.8
	HA	54 Lys	HD3	1865.0
	HA	55 Lys	HN	759.0
	HB2	55 Lys	HN	1840.0

55 Lys

	HN	55 Lys	HA	2973.0
	HN	55 Lys	HB2	4426.0
	HN	55 Lys	HB3	6352.0
	HN	56 Asn	HN	13680.0
	HN	56 Asn	HA	882.0
	HA	55 Lys	HB2	2353.0
	HA	56 Asn	HN	219.0
	HB2	56 Asn	HN	847.0
	HB2	57 Val	QG2	609.3
	HB2	74 Tyr	CZ	878.0*2
	HB2	75 Ile	QG2	3562.0
	HB3	56 Asn	HN	1512.0
	HB3	74 Tyr	CZ	140.5*2
	HB3	75 Ile	HA	388.0
	HB3	75 Ile	QG2	995.0

56 Asn

	HN	56 Asn	HA	4358.0
	HN	56 Asn	HB2	1225.0
	HN	56 Asn	HB3	972.0
	HN	56 Asn	HD22	766.0
	HN	57 Val	QG1	341.0

	HA	56	Asn	HB2	4468.0
	HA	56	Asn	HB3	2557.0
	HA	56	Asn	HD21	1521.0
	HA	56	Asn	HD22	341.0
	HA	57	Val	HN	2810.0
	HA	57	Val	QG1	197.0
	HB2	56	Asn	HD21	1364.0
	HB2	56	Asn	HD22	776.0
	HB3	56	Asn	HD21	882.0
	HB3	56	Asn	HD22	127.0
57 Val					
	HN	57	Val	HA	3073.0
	HN	57	Val	HB	985.0
	HN	57	Val	QG1	3949.0
	HN	57	Val	QG2	2815.0
	HN	58	Leu	HN	684.0
	HA	57	Val	HB	2827.0
	HA	57	Val	QG1	1603.0
	HA	57	Val	QG2	2143.0
	HA	58	Leu	HN	15220.0
	HB	57	Val	QG1	20430.0
	HB	57	Val	QG2	6099.0
	HB	58	Leu	HN	445.0
	HB	59	Trp	HZ2	238.0
	QG1	58	Leu	HN	2689.0
	QG1	59	Trp	HA	714.6
	QG1	59	Trp	HE3	598.5
	QG1	59	Trp	HZ3	3531.0
	QG1	59	Trp	HH2	455.0
	QG1	63	Asn	HD21	2032.0
	QG1	63	Asn	HD22	1553.0
	QG1	74	Tyr	CG	252.5*2
	QG1	74	Tyr	CZ	655.5*2
	QG2	58	Leu	HN	1490.0
	QG2	59	Trp	HA	553.0
	QG2	59	Trp	HE3	1025.0
	QG2	59	Trp	HE1	246.0
	QG2	59	Trp	HZ3	1256.0
	QG2	59	Trp	HZ2	606.0
	QG2	59	Trp	HH2	1214.0
	QG2	63	Asn	HB2	599.4
	QG2	63	Asn	HD21	372.0
	QG2	63	Asn	HD22	963.0
	QG2	74	Tyr	CG	109.8*2
	QG2	74	Tyr	CZ	2302.2*2
	QG2	75	Ile	QD1	2318.0
58 Leu					
	HN	58	Leu	HA	468.0
	HN	58	Leu	HB2	5845.0
	HN	58	Leu	HB3	7496.0
	HN	58	Leu	QD1	363.0
	HN	58	Leu	QD2	839.0
	HN	63	Asn	HD22	192.0
	HA	58	Leu	HB2	2906.0
	HA	58	Leu	HG	295.0
	HA	58	Leu	QD1	7343.0
	HA	58	Leu	QD2	1786.0
	HA	59	Trp	HN	4526.0
	HB2	58	Leu	QD1	2650.0

	HB2	59 Trp	HN	170.0
	HB3	58 Leu	QD1	2719.0
	HB3	58 Leu	QD2	2599.0
	HG	58 Leu	QD1	12100.0
	HG	58 Leu	QD2	3607.0
	HG	59 Trp	HN	107.0
	QD1	59 Trp	HN	1776.0
	QD2	59 Trp	HN	373.0
59 Trp				
	HN	59 Trp	HA	853.0
	HN	59 Trp	HB2	2596.0
	HN	59 Trp	HB3	847.0
	HN	59 Trp	HD1	1378.0
	HA	59 Trp	HB2	2230.2
	HA	59 Trp	HB3	6675.0
	HA	59 Trp	HE3	7222.0
	HA	60 Asp	HN	2344.0
	HA	63 Asn	HB2	1086.0
	HA	63 Asn	HD21	117.0
	HA	63 Asn	HD22	762.0
	HA	64 Met	HN	274.0
	HA	64 Met	QE	99.9
	HB2	64 Met	QE	903.0
	HB3	59 Trp	HD1	703.0
	HB3	59 Trp	HE3	612.0
	HD1	59 Trp	HE1	2791.0
	HE3	59 Trp	HZ3	2877.0
	HE3	59 Trp	HH2	126.0
	HE3	60 Asp	HN	1265.0
	HE3	64 Met	HN	631.0
	HE3	64 Met	HB2	409.5
	HE3	64 Met	HB3	1469.0
	HE3	64 Met	QE	897.0
	HE1	59 Trp	HZ2	5605.0
	HZ3	59 Trp	HH2	3253.0
	HZ3	64 Met	HB2	289.8
	HZ3	64 Met	HB3	174.6
	HZ3	67 Tyr	HN	590.0
	HZ3	67 Tyr	HB2	1075.0
	HZ3	67 Tyr	HB3	948.0
	HZ2	59 Trp	HH2	2839.0
	HZ2	75 Ile	QD1	1816.0
	HH2	67 Tyr	HB2	175.0
	HH2	67 Tyr	HB3	753.0
	HH2	74 Tyr	CG	260.5*2
	HH2	75 Ile	QD1	2554.0
60 Asp				
	HN	60 Asp	HB3	897.0
	HN	63 Asn	HD22	242.0
	HN	64 Met	HN	532.0
	HA	60 Asp	HB2	8589.0
	HA	60 Asp	HB3	1054.0
	HA	61 Glu	HN	1192.0
	HB2	61 Glu	HN	1499.0
	HB3	61 Glu	HN	3620.0
	HB3	62 Asn	HN	992.0
61 Glu				
	HN	61 Glu	HA	1555.0

	HN	61 Glu	HB2	1309.0
	HN	61 Glu	HB3	2877.0
	HN	62 Asn	HN	1245.0
	HA	61 Glu	HB2	4609.0
	HA	61 Glu	HB3	2847.0
	HA	62 Asn	HN	1323.0
	HA	64 Met	HN	444.0
	HA	95 Ile	QG2	2924.0
	HB2	62 Asn	HN	863.0
	HB2	95 Ile	QG2	1582.0
	HB3	62 Asn	HN	3801.0
	HB3	95 Ile	QG2	2427.0
62 Asn				
	HN	62 Asn	HA	3164.0
	HN	62 Asn	HB2	2086.0
	HN	62 Asn	HB3	3203.0
	HN	62 Asn	HD21	797.0
	HN	63 Asn	HN	4389.0
	HN	63 Asn	HB3	694.0
	HN	64 Met	HN	369.0
	HA	62 Asn	HB2	3331.0
	HA	62 Asn	HB3	2444.4
	HA	63 Asn	HN	629.0
	HA	65 Ser	HN	1362.0
	HB2	62 Asn	HD21	1444.0
	HB2	63 Asn	HN	956.0
	HB3	62 Asn	HD21	1582.0
	HB3	63 Asn	HN	1488.0
63 Asn				
	HN	63 Asn	HA	881.0
	HN	63 Asn	HB2	859.0
	HN	63 Asn	HB3	1181.0
	HN	63 Asn	HD21	111.0
	HN	64 Met	HN	3442.0
	HN	65 Ser	HN	272.0
	HN	66 Glu	HN	107.0
	HA	63 Asn	HB2	4584.0
	HA	63 Asn	HB3	2630.0
	HA	64 Met	HN	250.0
	HA	66 Glu	HN	1879.0
	HA	66 Glu	HB2	2070.9
	HA	66 Glu	HB3	2146.5
	HA	67 Tyr	HN	440.0
	HB2	63 Asn	HD21	2411.0
	HB2	63 Asn	HD22	1367.0
	HB3	63 Asn	HD21	929.0
	HB3	63 Asn	HD22	541.0
64 Met				
	HN	64 Met	HB2	3600.0
	HN	64 Met	HB3	4074.0
	HN	64 Met	QE	473.0
	HN	65 Ser	HN	1735.0
	HN	66 Glu	HN	384.0
	HB2	65 Ser	HN	707.0
	HB3	64 Met	QE	1821.0
	HB3	65 Ser	HN	773.0
	HB3	95 Ile	QG2	890.0

65 Ser

HN	65 Ser	HA	497.0
HN	95 Ile	QD1	1056.0
HA	66 Glu	HN	752.0
HA	68 Leu	HN	1268.0
HA	68 Leu	HG	1189.0
HA	95 Ile	QD1	5501.0

66 Glu

HN	66 Glu	HA	1097.0
HN	66 Glu	HB2	2198.0
HN	66 Glu	HB3	1065.0
HN	67 Tyr	HN	3263.0
HN	68 Leu	HN	322.0
HA	66 Glu	HB2	1629.0
HA	66 Glu	HB3	1603.0
HA	67 Tyr	HN	351.0
HB2	67 Tyr	HN	2494.0
HB2	74 Tyr	CG	186.5*2
HB2	74 Tyr	CZ	368.5*2
HB3	67 Tyr	HN	212.0
HB3	74 Tyr	CG	484.5*2
HB3	74 Tyr	CZ	143.6*2

67 Tyr

HN	67 Tyr	HA	770.0
HN	67 Tyr	HB2	2390.0
HN	67 Tyr	HB3	2675.0
HN	74 Tyr	CZ	144.5*2
HA	68 Leu	HN	176.0
HA	74 Tyr	HB2	2382.0
HA	74 Tyr	CG	876.5*2
HB2	67 Tyr	HD2	1891.8
HB2	68 Leu	HN	2709.0
HB3	67 Tyr	HD2	855.0
HD1	67 Tyr	HE2	4827.0
HD1	68 Leu	HB2	197.1
HD2	74 Tyr	HB2	310.5

68 Leu

HN	68 Leu	HA	3415.0
HN	68 Leu	HB2	6708.0
HN	68 Leu	HB3	1781.0
HN	68 Leu	HG	2011.0
HN	68 Leu	QD1	1626.0
HN	68 Leu	QD2	2382.0
HN	69 Thr	HN	574.0
HA	68 Leu	HB2	19180.0
HA	68 Leu	HG	174.0
HA	68 Leu	QD1	7097.0
HA	71 Pro	HG2	1092.6
HA	82 Phe	CZ	530.1*2
HB2	68 Leu	QD1	1465.0
HB2	69 Thr	HN	398.0
HB3	68 Leu	HG	3606.0
HB3	68 Leu	QD1	4185.0
HB3	82 Phe	CZ	506.7*2
HB3	85 Leu	HN	409.0
HG	68 Leu	QD1	7805.0
HG	68 Leu	QD2	7413.0
QD1	80 Met	QE	5365.0

	QD1	82 Phe	CZ	380.5*2
	QD1	82 Phe	HZ	67.5
	QD1	94 Leu	QD1	1461.6
	QD1	95 Ile	HG12	652.5
	QD2	71 Pro	HG2	707.4
	QD2	80 Met	QE	431.1
	QD2	91 Arg	HA	1642.5
69 Thr				
	HN	69 Thr	HA	598.0
	HN	69 Thr	HB	683.0
	HN	69 Thr	QG2	1235.0
	HN	70 Asn	HN	2277.0
	HN	71 Pro	HD3	967.0
	HA	69 Thr	HB	7494.0
	HA	69 Thr	QG2	1979.0
	HA	70 Asn	HN	655.0
	HA	85 Leu	HN	461.0
	HB	69 Thr	QG2	2250.0
	HB	70 Asn	HN	1025.0
	QG2	70 Asn	HB2	3904.0
	QG2	70 Asn	HB3	4226.0
	QG2	86 Lys	HA	762.0
70 Asn				
	HN	70 Asn	HA	664.0
	HN	70 Asn	HB2	4034.0
	HN	70 Asn	HB3	894.0
	HN	71 Pro	HG3	118.0
	HN	71 Pro	HD2	939.0
	HN	71 Pro	HD3	742.0
	HA	70 Asn	HB2	5350.0
	HA	70 Asn	HB3	3899.0
	HA	71 Pro	HD3	3088.0
	HA	73 Lys	HN	1131.0
	HB2	73 Lys	HB3	1069.0
71 Pro				
	HB2	71 Pro	HD2	939.0
	HB2	72 Tml	HN	2644.0
	HB2	80 Met	QE	916.0
	HB2	82 Phe	CG	893.5*2
	HG2	71 Pro	HD2	2427.0
	HG2	71 Pro	HD3	3218.0
	HG2	80 Met	QE	3219.0
	HG2	82 Phe	CG	739.0*2
	HG2	82 Phe	CZ	59.8*2
	HG2	84 Gly	HA2	680.0
	HG3	71 Pro	HD2	633.0
	HG3	71 Pro	HD3	1406.7
	HG3	80 Met	HG3	185.4
	HG3	80 Met	QE	2761.2
	HG3	82 Phe	CG	2591.0*2
	HG3	84 Gly	HA2	679.0
	HD2	72 Tml	HN	2034.0
	HD2	80 Met	QE	54.0
	HD2	82 Phe	CG	231.5*2
	HD2	82 Phe	CZ	110.7*2
	HD3	80 Met	QE	779.4
	HD3	82 Phe	CG	406.0*2
	HD3	82 Phe	CZ	58.0*2

72 Tml

	HN	72 Tml	HA	1455.0
	HN	72 Tml	HB2	4867.0
	HN	72 Tml	HB3	1077.0
	HN	72 Tml	HG2	1395.0
	HN	73 Lys	HN	3183.0
	HN	78 Thr	QG2	403.0
	HA	72 Tml	HB2	1996.0
	HA	72 Tml	HB3	2293.0
	HA	72 Tml	HG2	1745.0
	HA	72 Tml	HE2	625.0
	HA	73 Lys	HN	2036.0
	HA	75 Ile	HN	875.0
	HA	77 Gly	HN	350.0
	HA	78 Thr	QG2	3163.0
	HB2	73 Lys	HA	254.0
	HB3	72 Tml	HE3	4555.0
	HG2	72 Tml	HE2	1136.0
	HG2	72 Tml	HE3	5062.5
	HG2	72 Tml	QQH	3843.9
	HG2	78 Thr	HN	689.0
	HE3	81 Ala	HA	1369.0
	QQH	81 Ala	HA	3346.2
	QQH	81 Ala	QB	3870.0
	QQH	82 Phe	HN	304.0

73 Lys

	HN	73 Lys	HA	3382.0
	HN	73 Lys	HB3	12610.0
	HN	74 Tyr	HN	11850.0
	HN	75 Ile	HN	822.0
	HA	73 Lys	HB3	3720.0
	HA	74 Tyr	HN	880.0
	HB3	74 Tyr	HN	1068.0

74 Tyr

	HN	74 Tyr	HA	768.0
	HN	74 Tyr	HB2	2298.0
	HN	74 Tyr	HB3	2702.0
	HN	75 Ile	HN	4561.0
	HA	74 Tyr	HB2	1190.0
	HA	74 Tyr	HB3	569.0
	HA	74 Tyr	CG	2536.5*2
	HA	74 Tyr	CZ	220.9*2
	HA	75 Ile	HN	464.0
	HB2	74 Tyr	CG	2799.5*2
	HB2	75 Ile	HN	1815.0
	HB3	74 Tyr	CG	1031.5*2
	HB3	74 Tyr	CZ	488.5*2
	HB3	75 Ile	HN	1616.0
	CG	74 Tyr	CZ	3085.0*2*2
	CG	75 Ile	HN	239.0*2
	CG	75 Ile	QG2	279.4*2
	CZ	75 Ile	QD1	766.0*2

75 Ile

	HN	75 Ile	HA	1180.0
	HN	75 Ile	HB	1273.0
	HN	75 Ile	QG2	396.0
	HN	75 Ile	QD1	238.0

	HA	75 Ile	HB	758.0
	HA	75 Ile	QG2	1915.0
	HA	76 Pro	HD2	3845.0
	HB	75 Ile	QG2	5656.0
	HB	75 Ile	QD1	5320.0
	HB	78 Thr	HN	425.0
	HB	78 Thr	HB	573.0
	HB	78 Thr	QG2	4325.0
	QG2	75 Ile	QD1	7427.7
	QG2	78 Thr	HN	1159.0
	QG2	78 Thr	HA	1262.7
	QG2	78 Thr	HB	1859.0
76 Pro				
	HA	76 Pro	HB2	6993.9
	HA	76 Pro	HB3	6335.0
	HA	76 Pro	HD3	6138.9
	HA	77 Gly	HN	365.0
	HB2	77 Gly	HN	680.0
	HG2	76 Pro	HD2	6427.0
	HG2	76 Pro	HD3	4945.0
	HG3	76 Pro	HD3	987.3
77 Gly				
	HN	77 Gly	HA1	961.0
	HN	78 Thr	HN	686.0
	HN	78 Thr	QG2	833.0
	HA1	78 Thr	HN	1144.0
	HA2	78 Thr	HN	287.0
78 Thr				
	HN	78 Thr	HA	3566.0
	HN	78 Thr	HB	1387.0
	HN	78 Thr	QG2	6887.0
	HA	78 Thr	HB	10494.0
	HA	78 Thr	QG2	3101.4
	HA	79 Lys	HN	3364.0
	HA	80 Met	HN	1279.0
	HA	80 Met	HB3	533.7
	HB	78 Thr	QG2	4737.0
	QG2	79 Lys	HN	1132.0
	QG2	80 Met	HN	2891.0
	QG2	80 Met	HB2	1020.6
	QG2	80 Met	HB3	3866.0
	QG2	80 Met	HG2	233.1
	QG2	81 Ala	HN	307.0
79 Lys				
	HN	79 Lys	HA	556.0
	HN	80 Met	HN	1185.0
	HA	80 Met	HN	514.0
80 Met				
	HN	80 Met	HA	939.0
	HN	80 Met	HB2	2832.0
	HN	80 Met	HB3	3569.0
	HN	80 Met	HG2	436.0
	HN	80 Met	HG3	327.0
	HN	81 Ala	HN	645.0
	HA	80 Met	HB2	2710.0
	HA	80 Met	HB3	1688.0

	HA	80	Met	HG2	3120.0
	HA	80	Met	HG3	1645.0
	HA	80	Met	QE	359.1
	HA	81	Ala	HN	5784.0
	HB2	80	Met	HG2	2262.0
	HB2	80	Met	HG3	2364.0
	HB2	80	Met	QE	1325.0
	HB2	81	Ala	HN	392.0
	HB3	80	Met	HG2	2677.0
	HB3	80	Met	HG3	2879.0
	HB3	80	Met	QE	868.0
	HB3	81	Ala	HN	239.0
	HB3	81	Ala	HA	190.8
	HG2	80	Met	QE	3933.0
	HG2	81	Ala	HN	1151.0
	HG2	81	Ala	QB	238.5
	HG2	82	Phe	HN	336.0
	HG2	82	Phe	HB2	722.0
	HG2	82	Phe	HB3	528.0
	HG2	82	Phe	CG	62.0*2
	HG3	80	Met	QE	6057.0
	HG3	81	Ala	HN	287.0
	HG3	82	Phe	HN	397.0
	HG3	82	Phe	HB2	1256.0
	HG3	82	Phe	HB3	2495.0
	HG3	82	Phe	CG	126.4*2
	QE	82	Phe	HN	534.0
	QE	82	Phe	HA	182.7
	QE	82	Phe	HB2	4330.0
	QE	82	Phe	HB3	2507.0
	QE	82	Phe	CG	2981.5*2
	QE	82	Phe	CZ	303.0*2
81	Ala				
	HN	81	Ala	HA	1875.0
	HN	81	Ala	QB	12520.0
	HN	82	Phe	HN	616.0
	HA	81	Ala	QB	10660.0
	HA	82	Phe	HN	4837.0
	QB	82	Phe	HN	1449.0
82	Phe				
	HN	82	Phe	HA	1455.3
	HN	82	Phe	HB2	1431.0
	HN	82	Phe	HB3	1325.0
	HN	82	Phe	CG	703.0*2
	HA	82	Phe	HB2	1721.7
	HA	82	Phe	HB3	1224.0
	HA	82	Phe	CG	1144.8*2
	HA	82	Phe	CZ	117.4*2
	HB2	82	Phe	CG	3431.5*2
	HB3	82	Phe	CG	1859.5*2
	CG	82	Phe	CZ	2962.5*2*2
	CG	84	Gly	HA1	258.0*2
	CZ	84	Gly	HA1	351.0*2
	CZ	84	Gly	HA2	726.3*2
	CZ	85	Leu	HN	1259.5*2
	CZ	85	Leu	HB2	434.0*2
	CZ	85	Leu	HG	1550.0*2
	CZ	85	Leu	QD1	1598.5*2
	CZ	85	Leu	QD2	955.0*2

	HZ	85 Leu	HN	704.0
	HZ	85 Leu	HG	3851.0
	HZ	85 Leu	QD1	2402.0
	HZ	85 Leu	QD2	3492.0
84 Gly				
	HN	84 Gly	HA1	1180.0
	HN	85 Leu	HN	446.0
	HA1	85 Leu	HN	2821.0
	HA2	85 Leu	HN	900.0
85 Leu				
	HN	85 Leu	HB2	3761.0
	HN	85 Leu	HB3	1746.0
	HN	85 Leu	HG	3339.0
	HN	85 Leu	QD1	396.0
	HN	85 Leu	QD2	1360.0
	HA	85 Leu	HB3	1487.7
	HA	85 Leu	QD1	802.8
	HA	85 Leu	QD2	2833.2
	HB2	87 Lys	HN	275.0
	HB3	85 Leu	QD1	1900.0
	HG	85 Leu	QD1	4771.0
	HG	85 Leu	QD2	2164.0
	QD1	90 Asp	HB3	2184.3
	QD1	91 Arg	HA	699.0
	QD1	94 Leu	QD1	2411.0
	QD2	94 Leu	QD1	2451.0
86 Lys				
	HN	86 Lys	HA	1088.0
	HN	86 Lys	HB2	1714.0
	HN	87 Lys	HN	1465.0
	HA	87 Lys	HN	282.0
	HB2	87 Lys	HN	1103.0
87 Lys				
	HN	87 Lys	HA	705.0
	HN	87 Lys	HB2	3122.0
	HN	87 Lys	HB3	1367.0
	HN	87 Lys	HG2	2536.0
	HN	90 Asp	HB2	455.0
	HA	87 Lys	HB2	2303.1
	HA	87 Lys	HB3	3467.7
	HA	87 Lys	HG2	2309.4
	HB2	90 Asp	HN	2707.0
	HB3	89 Lys	HN	2443.0
	HB3	90 Asp	HN	1261.0
	HB3	90 Asp	HB2	934.0
	HB3	90 Asp	HB3	1166.0
88 Glu				
	HN	88 Glu	HB2	1451.0
	HN	88 Glu	HB3	1526.0
	HN	89 Lys	HN	1552.0
	HA	88 Glu	HB2	1543.0
	HA	88 Glu	HB3	3717.0
	HA	91 Arg	HN	1319.0
	HA	91 Arg	HB2	3163.0
	HA	91 Arg	HB3	169.0
	HA	92 Asn	HN	431.0

	HB2	89	Lys	HN	3471.0
	HB3	89	Lys	HN	1232.0
89 Lys					
	HN	89	Lys	HA	3704.0
	HN	89	Lys	HB2	6540.0
	HN	89	Lys	HB3	2053.0
	HN	89	Lys	HG2	1393.0
	HN	89	Lys	HG3	1593.0
	HN	90	Asp	HN	2388.0
	HN	91	Arg	HN	539.0
	HA	89	Lys	HB2	5147.0
	HA	89	Lys	HB3	6838.2
	HA	89	Lys	HG3	1244.0
	HA	90	Asp	HN	905.0
	HA	92	Asn	HD22	209.0
	HB2	90	Asp	HN	6110.0
	HB2	91	Arg	HN	545.0
	HB3	90	Asp	HN	609.0
	HG2	90	Asp	HN	571.0
	HG3	90	Asp	HN	1134.0
90 Asp					
	HN	90	Asp	HA	3811.0
	HN	90	Asp	HB2	2722.0
	HN	90	Asp	HB3	4817.0
	HN	91	Arg	HN	5507.0
	HN	91	Arg	HG3	891.0
	HN	92	Asn	HN	981.0
	HA	90	Asp	HB2	2919.0
	HA	90	Asp	HB3	4864.5
	HA	91	Arg	HN	451.0
	HB2	91	Arg	HN	1767.0
	HB3	91	Arg	HN	1441.0
91 Arg					
	HN	91	Arg	HA	1951.0
	HN	91	Arg	HB2	1787.0
	HN	91	Arg	HB3	1356.0
	HN	91	Arg	HG2	914.0
	HN	91	Arg	HG3	1393.0
	HN	92	Asn	HN	4430.0
	HN	94	Leu	HN	194.0
	HA	91	Arg	HB2	1878.0
	HA	91	Arg	HB3	325.0
	HA	91	Arg	HG2	4070.7
	HA	91	Arg	HG3	568.0
	HA	92	Asn	HN	420.0
	HA	94	Leu	HN	276.0
	HA	94	Leu	HB3	1896.0
	HB2	91	Arg	HG2	2332.0
	HB2	91	Arg	HG3	37960.0
	HB2	92	Asn	HN	4188.0
	HB3	91	Arg	HG2	3527.0
	HB3	92	Asn	HN	641.0
	HG3	92	Asn	HN	828.0
92 Asn					
	HN	92	Asn	HA	1780.0
	HN	92	Asn	HB2	6260.0
	HN	92	Asn	HB3	639.0

	HN	92 Asn	HD21	415.0
	HN	92 Asn	HD22	134.0
	HA	92 Asn	HB2	3861.0
	HA	92 Asn	HB3	3987.0
	HB2	92 Asn	HD21	1387.0
	HB2	92 Asn	HD22	679.0
	HB2	93 Asp	HN	2666.0
	HB3	92 Asn	HD21	1198.0
	HB3	93 Asp	HN	591.0
93 Asp				
	HN	93 Asp	HA	2215.0
	HN	93 Asp	HB2	3191.0
	HN	93 Asp	HB3	1201.0
	HN	94 Leu	HN	4638.0
	HA	93 Asp	HB2	3289.0
	HA	93 Asp	HB3	7688.7
	HB2	94 Leu	HN	1420.0
	HB2	94 Leu	QD1	858.0
	HB2	94 Leu	QD2	1818.0
	HB3	94 Leu	HN	2196.0
94 Leu				
	HN	94 Leu	HA	1951.0
	HN	94 Leu	HB2	4229.0
	HN	94 Leu	HB3	3440.0
	HN	94 Leu	QD1	240.0
	HN	95 Ile	HN	1126.0
	HA	94 Leu	HB2	6452.0
	HA	94 Leu	HB3	2730.0
	HA	94 Leu	QD1	3077.0
	HA	97 Tyr	HN	1546.0
	HA	97 Tyr	CG	135.9*2
	HA	98 Leu	QD1	303.0
	HB2	94 Leu	QD1	21480.0
	HB2	94 Leu	QD2	1291.0
	HB2	95 Ile	HN	530.0
	HB3	94 Leu	QD1	3579.0
	HB3	94 Leu	QD2	1667.0
	HB3	95 Ile	HN	2075.0
	QD1	95 Ile	HN	3453.0
	QD1	97 Tyr	CG	631.3*2
	QD1	98 Leu	HN	853.0
	QD1	98 Leu	QD1	839.0
	QD2	97 Tyr	CG	642.5*2
	QD2	97 Tyr	CZ	364.0*2
95 Ile				
	HN	95 Ile	HA	1590.0
	HN	95 Ile	HB	3322.0
	HN	95 Ile	QG2	1425.0
	HN	95 Ile	HG12	4014.0
	HN	95 Ile	QD1	3970.0
	HN	96 Thr	HN	2685.0
	HN	97 Tyr	HN	651.0
	HA	95 Ile	HB	781.0
	HA	95 Ile	QG2	2417.0
	HA	95 Ile	HG12	1688.0
	HA	98 Leu	HN	1103.0
	HA	98 Leu	HB2	469.0
	HA	98 Leu	HB3	1273.0
	HA	98 Leu	QD1	1618.0

	HB	95	Ile	QG2	4454.0
	HB	95	Ile	QD1	11250.0
	HB	96	Thr	HN	1362.0
	QG2	95	Ile	HG12	2311.0
	QG2	95	Ile	QD1	12370.0
	QG2	96	Thr	HN	1368.0
	QG2	96	Thr	HA	736.0
	QG2	99	Lys	HN	178.0
	HG12	95	Ile	QD1	15680.0

96 Thr

	HN	96	Thr	HA	1719.0
	HN	96	Thr	HB	4377.0
	HN	96	Thr	QG2	267.0
	HN	97	Tyr	HN	3284.0
	HN	98	Leu	HN	61.0
	HN	98	Leu	HB3	757.0
	HA	96	Thr	HB	6800.4
	HA	96	Thr	QG2	10230.0
	HA	97	Tyr	HN	241.0
	HA	98	Leu	HN	344.0
	HA	99	Lys	HN	667.0
	HB	96	Thr	QG2	2606.0
	HB	97	Tyr	HN	2601.0
	QG2	97	Tyr	HN	620.0
	QG2	97	Tyr	HA	461.0

97 Tyr

	HN	97	Tyr	HA	942.0
	HN	97	Tyr	HB2	1615.0
	HN	97	Tyr	HB3	1388.0
	HN	98	Leu	HN	4633.0
	HN	99	Lys	HN	859.0
	HA	97	Tyr	HB3	2159.0
	HA	97	Tyr	CG	1826.1*2
	HA	98	Leu	HN	765.0
	HB2	97	Tyr	CZ	342.9*2
	HB2	98	Leu	HN	1065.0
	HB3	97	Tyr	CG	1685.2*2
	HB3	98	Leu	HN	1196.0
	CG	97	Tyr	CZ	1181.2*2*2
	CG	98	Leu	HA	528.8*2
	CG	98	Leu	HB3	2107.3*2
	CG	98	Leu	QD1	163.3*2
	CG	98	Leu	QD2	509.4*2
	CG	101	Ala	QB	346.0*2
	CZ	101	Ala	QB	425.7*2

98 Leu

	HN	98	Leu	HA	3131.0
	HN	98	Leu	HB2	4877.0
	HN	98	Leu	HB3	3607.0
	HN	98	Leu	QD1	941.0
	HN	98	Leu	QD2	890.0
	HN	99	Lys	HN	4328.0
	HN	100	Lys	HN	117.0
	HA	98	Leu	QD1	6542.0
	HA	98	Leu	QD2	3767.0
	HA	99	Lys	HN	666.0
	HA	100	Lys	HN	897.0
	HA	101	Ala	HN	2424.0

HA	101	Ala	QB	7928.0
HB2	98	Leu	QD1	1868.0
HB2	98	Leu	QD2	9999.0
HB2	99	Lys	HN	4057.0
HB3	98	Leu	QD1	9002.0
HB3	99	Lys	HN	2992.0
QD1	99	Lys	HN	208.0

99 Lys

HN	99	Lys	HA	3233.0
HN	99	Lys	HB2	4464.0
HN	99	Lys	HB3	5084.0
HN	100	Lys	HN	2990.0
HN	101	Ala	HN	453.0
HA	99	Lys	HB2	4145.0
HA	99	Lys	HB3	5088.0
HA	100	Lys	HN	1477.0
HB3	100	Lys	HN	4786.0

100 Lys

HN	100	Lys	HA	3695.0
HN	100	Lys	HB2	17810.0
HN	100	Lys	HB3	4322.0
HN	101	Ala	HN	9652.0
HN	102	Ser	HN	1044.0
HA	100	Lys	HB2	16420.0
HA	100	Lys	HB3	1708.0
HA	101	Ala	HN	1695.0
HA	103	Glu	HN	333.0
HB2	101	Ala	HN	3524.0
HB3	101	Ala	HN	1060.0

101 Ala

HN	101	Ala	HA	4550.0
HN	101	Ala	QB	14250.0
HN	102	Ser	HN	4460.0
HN	103	Glu	HN	1524.0
HA	101	Ala	QB	13910.0
HA	102	Ser	HN	1098.0
QB	102	Ser	HN	3498.0

102 Ser

HN	102	Ser	HA	680.0
HN	103	Glu	HN	4559.0
HA	103	Glu	HN	629.0

103 Glu

HN	103	Glu	HA	2687.0
HN	103	Glu	HB2	1131.0
HN	103	Glu	HB3	7087.0
HA	103	Glu	HB2	439.0
HA	103	Glu	HB3	6072.0

Part III: *Irrelevant NOESY constraints*

HN	Glu	-4	HN	Phe	-3
HN	Phe	-3	HA	Phe	-3
HN	Phe	-3	HA	Phe	-3
HN	Phe	-3	HB3	Phe	-3
HA	Phe	-3	HB2	Phe	-3

HA	Phe	-3	-	HB2	Phe	-3
HA	Phe	-3	-	HB3	Phe	-3
HA	Phe	-3	-	HB3	Phe	-3
HA	Phe	-3	-	CG	Phe	-3
HA	Phe	-3	-	CG	Phe	-3
HA	Phe	-3	-	HN	Lys	-2
HA	Phe	-3	-	HN	Lys	-2
HA	Phe	-3	-	HD22	Asn	92
HB2	Phe	-3	-	CG	Phe	-3
HB2	Phe	-3	-	CG	Phe	-3
HB2	Phe	-3	-	CZ	Phe	-3
HB2	Phe	-3	-	CZ	Phe	-3
HB3	Phe	-3	-	CG	Phe	-3
HB3	Phe	-3	-	CG	Phe	-3
CG	Phe	-3	-	CZ	Phe	-3
CG	Phe	-3	-	CZ	Phe	-3
CG	Phe	-3	-	HA	Lys	-2
CG	Phe	-3	-	HB2	Glu	61
CG	Phe	-3	-	HB3	Glu	61
CG	Phe	-3	-	HA	Asn	92
CG	Phe	-3	-	HB	Ile	95
CG	Phe	-3	-	QG2	Ile	95
CG	Phe	-3	-	QD1	Ile	95
CG	Phe	-3	-	HN	Thr	96
CZ	Phe	-3	-	HZ	Phe	-3
CZ	Phe	-3	-	HZ	Phe	-3
CZ	Phe	-3	-	HB3	Glu	61
CZ	Phe	-3	-	HB3	Asn	92
CZ	Phe	-3	-	HN	Ile	95
CZ	Phe	-3	-	HA	Ile	95
CZ	Phe	-3	-	HB	Ile	95
CZ	Phe	-3	-	QG2	Ile	95
CZ	Phe	-3	-	QD1	Ile	95
CZ	Phe	-3	-	HN	Thr	96
HZ	Phe	-3	-	HA	Ala	-1
HZ	Phe	-3	-	QB	Ala	-1
HZ	Phe	-3	-	HN	Gly	1
HZ	Phe	-3	-	HB	Ile	95
HZ	Phe	-3	-	QG2	Ile	95
HZ	Phe	-3	-	HN	Thr	96
HZ	Phe	-3	-	HA	Thr	96
HN	Lys	-2	-	HA	Lys	-2
HN	Lys	-2	-	HA	Lys	-2
HN	Lys	-2	-	HB2	Lys	-2
HN	Lys	-2	-	HB3	Lys	-2
HN	Lys	-2	-	HB3	Asn	92
HN	Lys	-2	-	HD21	Asn	92
HN	Lys	-2	-	HD22	Asn	92
HA	Lys	-2	-	HB2	Lys	-2
HA	Lys	-2	-	HB2	Lys	-2
HA	Lys	-2	-	HB3	Lys	-2
HA	Lys	-2	-	HB3	Lys	-2
HA	Lys	-2	-	HN	Ala	-1
HB2	Lys	-2	-	HN	Ala	-1
HB3	Lys	-2	-	HN	Ala	-1
HN	Ala	-1	-	HA	Ala	-1
HN	Ala	-1	-	HA	Ala	-1
HN	Ala	-1	-	QB	Ala	-1
HA	Ala	-1	-	QB	Ala	-1
HA	Ala	-1	-	QB	Ala	-1
HA	Ala	-1	-	HN	Gly	1

HA	Ala	-1 - HB3	Asn	92
HA	Ala	-1 - QG2	Thr	96
QB	Ala	-1 - HN	Gly	1
HN	Gly	1 - HA1	Gly	1
HN	Gly	1 - HA1	Gly	1
HN	Gly	1 - HA2	Gly	1
HN	Gly	1 - HA2	Gly	1
HN	Gly	1 - HN	Ser	2
HN	Gly	1 - HA	Asp	93
HN	Gly	1 - QG2	Thr	96
HA1	Gly	1 - HN	Ser	2
HA1	Gly	1 - HA	Asp	93
HA2	Gly	1 - HN	Ser	2
HA2	Gly	1 - HN	Ser	2
HN	Ser	2 - HB2	Ser	2
HN	Ser	2 - HB3	Ser	2
HN	Ser	2 - HB3	Ser	2
HN	Ser	2 - HA	Asp	93
HN	Ser	2 - HB2	Asp	93
HA	Ser	2 - HB2	Ser	2
HA	Ser	2 - HB3	Ser	2
HA	Ala	3 - QB	Ala	3
HA	Ala	3 - QB	Ala	3
HA	Ala	3 - HN	Lys	4
HA	Ala	3 - HN	Gly	6
HA	Ala	3 - QG2	Thr	96
QB	Ala	3 - CG	Tyr	97
HN	Lys	4 - HA	Lys	4
HN	Lys	4 - HA	Lys	4
HA	Lys	4 - HN	Lys	5
HN	Lys	5 - HA	Lys	5
HN	Lys	5 - HA	Lys	5
HN	Lys	5 - HN	Gly	6
HA	Lys	5 - HN	Gly	6
HA	Lys	5 - HN	Gly	6
HA	Lys	5 - HN	Ala	7
HA	Lys	5 - HN	Thr	8
HN	Gly	6 - HA1	Gly	6
HN	Gly	6 - HA1	Gly	6
HN	Gly	6 - HA2	Gly	6
HN	Gly	6 - HA2	Gly	6
HN	Gly	6 - HN	Ala	7
HN	Gly	6 - QB	Ala	7
HN	Gly	6 - HB2	Asp	93
HN	Gly	6 - HB2	Tyr	97
HA1	Gly	6 - HN	Ala	7
HA1	Gly	6 - HN	Ala	7
HA1	Gly	6 - HN	Phe	10
HA1	Gly	6 - HB2	Asp	93
HA1	Gly	6 - HB3	Asp	93
HA2	Gly	6 - HN	Ala	7
HA2	Gly	6 - HN	Ala	7
HA2	Gly	6 - HN	Leu	9
HA2	Gly	6 - HB3	Tyr	97
HN	Ala	7 - HA	Ala	7
HN	Ala	7 - HA	Ala	7
HN	Ala	7 - QB	Ala	7
HN	Ala	7 - HN	Thr	8
HN	Ala	7 - HB2	Tyr	97
HA	Ala	7 - QB	Ala	7
HA	Ala	7 - QB	Ala	7

HA	Ala	7	-	HN	Thr 8
HA	Ala	7	-	HN	Thr 8
HA	Ala	7	-	HN	Phe 10
HA	Ala	7	-	HB2	Phe 10
HA	Ala	7	-	HB3	Phe 10
HA	Ala	7	-	HN	Lys 11
HA	Ala	7	-	CG	Tyr 97
QB	Ala	7	-	HN	Thr 8
QB	Ala	7	-	CG	Tyr 97
QB	Ala	7	-	CZ	Tyr 97
HN	Thr	8	-	HA	Thr 8
HN	Thr	8	-	HA	Thr 8
HN	Thr	8	-	HB	Thr 8
HN	Thr	8	-	QG2	Thr 8
HN	Thr	8	-	HN	Leu 9
HA	Thr	8	-	HB	Thr 8
HA	Thr	8	-	QG2	Thr 8
HA	Thr	8	-	HN	Leu 9
HA	Thr	8	-	HN	Leu 9
HA	Thr	8	-	HN	Lys 11
HA	Thr	8	-	HB2	Lys 11
HA	Thr	8	-	HB3	Lys 11
HB	Thr	8	-	QG2	Thr 8
HB	Thr	8	-	QG2	Thr 8
HB	Thr	8	-	HN	Leu 9
QG2	Thr	8	-	HN	Leu 9
HN	Leu	9	-	HA	Leu 9
HN	Leu	9	-	HA	Leu 9
HN	Leu	9	-	HB2	Leu 9
HN	Leu	9	-	HB3	Leu 9
HN	Leu	9	-	HN	Phe 10
HN	Leu	9	-	HN	Lys 11
HA	Leu	9	-	HB2	Leu 9
HA	Leu	9	-	HB2	Leu 9
HA	Leu	9	-	HB3	Leu 9
HA	Leu	9	-	HB3	Leu 9
HA	Leu	9	-	HG	Leu 9
HA	Leu	9	-	QD1	Leu 9
HA	Leu	9	-	QD2	Leu 9
HA	Leu	9	-	HN	Phe 10
HA	Leu	9	-	HN	Phe 10
HA	Leu	9	-	HG2	Arg 13
HB2	Leu	9	-	QD1	Leu 9
HB2	Leu	9	-	QD1	Leu 9
HB2	Leu	9	-	QD2	Leu 9
HB2	Leu	9	-	QD2	Leu 9
HB2	Leu	9	-	HN	Phe 10
HB2	Leu	9	-	QD1	Leu 94
HB3	Leu	9	-	HN	Phe 10
HB3	Leu	9	-	HA	Phe 10
HG	Leu	9	-	QD1	Leu 9
HG	Leu	9	-	QD1	Leu 9
HG	Leu	9	-	HN	Phe 10
QD1	Leu	9	-	HA	Asp 90
QD1	Leu	9	-	HB2	Asp 90
QD1	Leu	9	-	HB3	Asp 90
QD1	Leu	9	-	HN	Asp 93
QD1	Leu	9	-	HN	Leu 94
HN	Phe	10	-	HA	Phe 10
HN	Phe	10	-	HA	Phe 10
HN	Phe	10	-	HB2	Phe 10

HN	Phe	10	- HB3	Phe	10
HN	Phe	10	- HN	Lys	11
HN	Phe	10	- QD1	Leu	94
HN	Phe	10	- QD2	Leu	94
HA	Phe	10	- HB2	Phe	10
HA	Phe	10	- HB2	Phe	10
HA	Phe	10	- HB3	Phe	10
HA	Phe	10	- HB3	Phe	10
HA	Phe	10	- CG	Phe	10
HA	Phe	10	- CG	Phe	10
HA	Phe	10	- HN	Cys	14
HA	Phe	10	- QD1	Leu	94
HA	Phe	10	- QD2	Leu	94
HB2	Phe	10	- CG	Phe	10
HB2	Phe	10	- CG	Phe	10
HB2	Phe	10	- QD1	Leu	94
HB3	Phe	10	- CG	Phe	10
HB3	Phe	10	- CG	Phe	10
HB3	Phe	10	- HN	Lys	11
HB3	Phe	10	- QD1	Leu	94
HB3	Phe	10	- CG	Tyr	97
HB3	Phe	10	- CZ	Tyr	97
CG	Phe	10	- HE1	Phe	10
CG	Phe	10	- HE1	Phe	10
CG	Phe	10	- HE2	Phe	10
CG	Phe	10	- HE2	Phe	10
CG	Phe	10	- HN	Lys	11
CG	Phe	10	- HA	Lys	11
CG	Phe	10	- HB2	Leu	15
CG	Phe	10	- QD1	Leu	15
CG	Phe	10	- QD2	Leu	15
CG	Phe	10	- QD1	Leu	32
CG	Phe	10	- QD1	Leu	94
CG	Phe	10	- QD1	Leu	98
HE1	Phe	10	- HA	Leu	15
HE1	Phe	10	- HB2	Leu	15
HE1	Phe	10	- QD1	Leu	15
HE1	Phe	10	- QD2	Leu	15
HE1	Phe	10	- HA	Thr	19
HE1	Phe	10	- QG2	Val	20
HE1	Phe	10	- QD1	Leu	98
HZ	Phe	10	- HB2	Hes	18
HZ	Phe	10	- HB3	Hes	18
HZ	Phe	10	- HA	Thr	19
HZ	Phe	10	- QG1	Val	20
HZ	Phe	10	- QG2	Val	20
HZ	Phe	10	- QD1	Leu	32
HE2	Phe	10	- QD1	Leu	15
HE2	Phe	10	- QM1	Hes	18
HE2	Phe	10	- QG1	Val	20
HE2	Phe	10	- HG	Leu	32
HE2	Phe	10	- QD1	Leu	32
HE2	Phe	10	- QD2	Leu	98
HN	Lys	11	- HA	Lys	11
HN	Lys	11	- HA	Lys	11
HN	Lys	11	- HB2	Lys	11
HN	Lys	11	- HB3	Lys	11
HN	Lys	11	- HG3	Lys	11
HN	Lys	11	- HN	Thr	12
HN	Lys	11	- QD2	Leu	15
HA	Lys	11	- HB2	Lys	11